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16. ABSTRACT

The EKMA was evaluated by comparison with more complex models using common data bases for the San Francisco and Sacramento areas. The basic model used in the EKMA is a simple, moving-air-parcel, or trajectory, model that uses a detailed chemical mechanism for the surrogate propylene and butane hydrocarbons. Time-dependent, precursor-emission factors can be treated, along with expansion of the air parcel, but entrainment is treated by assuming that constant concentrations exist outside the parcel. This basic model is used to generate ozone isopleth diagrams for estimating ozone response to hydrocarbon and nitrogen oxide controls. The comparison study involved several levels of the EKMA system, from parts of the basic model to control strategy predictions. For the San Francisco area, the EKMA was compared with the LIRAQ model, which had been used for the 1979 AQMP. For the Sacramento area, the EKMA was compared with the SAI Airshed Model. When carefully applied, the EKMA produced results that typically agreed with the more complex models. However, the evaluation confirmed that care must be exercised in applying the model to situations involving wind shear, complex terrain features, and highly nonuniform emission densities, and that caution must be used in interpreting the results of model applications to situations involving these factors.

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Volume I: San Francisco/Sacramento

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32R/1

CONTENTS

DISCLAIMER..... ii

LIST OF ILLUSTRATIONS..... v

LIST OF TABLES..... vii

LIST OF EXHIBITS..... ix

1 INTRODUCTION..... 1

1.1 Background and Objectives..... 2

2 SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS..... 4

2.1 Summary..... 4

2.2 Conclusions..... 4

2.3 Recommendations..... 6

3 TRAJECTORY MODEL APPLICATIONS..... 9

3.1 San Francisco Applications..... 9

3.1.1 Model Definition..... 11

3.1.2 San Francisco Case Studies..... 18

3.1.3 Summary of Results for San Francisco Case Studies..... 31

3.2 Sacramento Applications..... 33

3.2.1 Model Definition..... 35

3.2.2 Sacramento Case Studies..... 43

3.2.3 Summary of Results for Sacramento Case Studies..... 51

4 SENSITIVITY STUDIES..... 57

4.1 The San Francisco Region..... 58

4.1.1 Initial Conditions..... 58

4.1.2 Mixing Heights..... 58

4.1.3 Emissions Vector..... 60

4.1.4 Model Size..... 60

4.2 The Sacramento Region..... 63

5 EKMA APPLICATIONS..... 66

5.1 Considerations Related to the Use of Isopleth Diagrams..... 67

5.1.1 Fixed Monitoring Sites..... 67
5.1.2 Uneven Changes in Emissions..... 67
5.1.3 Transported Pollutants..... 68

5.2 San Francisco Applications..... 68

5.2.1 Basic Comparisons between LIRAQ and EKMA..... 68
5.2.2 Further Investigations..... 74

5.3 Sacramento Application..... 86

REFERENCES..... 103

ILLUSTRATIONS

1	Trajectory 1 for 26 July 1973.....	19
2	Trajectory 2 for 26 July 1973.....	21
3	Trajectory 1 for 20 August 1973.....	23
4	Trajectory 2 for 20 August 1973.....	25
5	Trajectory 1 for 24 July 1974.....	27
6	Trajectory 2 for 24 July 1974.....	29
7	Locations of Monitoring Sites in the Sacramento Area.....	34
8	Trajectory Used for 24 August 1976.....	44
9	Comparison of Ozone between Station Observations and Model Predictions for City-Specific EKMA for 24 August 1976--Sacramento.....	49
10	Trajectory Used for 28 June 1976.....	50
11	Comparison of Ozone between Station Observations and Model Predictions for 28 June 1976--Sacramento.....	54
12	Effects of Inversion Heights on Maximum Ozone Produced: 26 June 1973, Trajectory 1.....	61
13	Effects of Wind Speed across San Francisco on Ozone Production: 26 June 1973.....	62
14	Effects of Trajectory Width on Maximum Ozone: 26 July 1973.....	64
15	Isopleth for 26 July 1973: Trajectory 1--HC/NO_x Ratio = 10/1.....	71

32R/1

16	Level III Trajectory for San Francisco--26 July 1973.....	72
17	Isopleth for 26 July 1973: Trajectory 1--HC/NO_x Ratio = 1/1.....	77
18	Isopleth for 26 July 1973: Trajectory 1--HC/NO_x Ratio = 100/1.....	78
19	Isopleth for 20 August 1973: Trajectory 1.....	80
20	Isopleth for 24 July 1974: Trajectory 2.....	81
21	New-Style Isopleth (1,1) for 26 July 1973: Trajectory 1.....	84
22	New-Style Isopleth (1,1) for 26 July 1973: Trajectory 1 Using the Carbon-Bond Mechanism.....	87
23	Map of the Hypothetical Urban Area Used to Study Transportation Control Strategies.....	88
24	Trajectory Used for the Control-Strategy Runs	90
25	City-Specific EKMA Isopleth for the Control-Strategy Calculations.....	95
26	Level III Trajectory for Hypothetical Region: 24 August 1976.....	100

TABLES

1	Input Data for the San Francisco Trajectories.....	14
2	Summary of Results for the San Francisco Case Studies.....	32
3	OZIPM/CBM Emissions and Mixing-Height Inputs for 24 August 1976.....	45
4	Initial Conditions for Calculations of 24 August 1976.....	46
5	Comparison of the SAI Trajectory Model and the OZIPM/CBM Calculations for 24 August 1976 for NO_x, PAR, ARO, and Ozone.....	47
6	Emission Rates and Mixing Heights Used in the OZIPM/CBM Calculations for 28 June 1976.....	52
7	Initial Conditions Used in the City-Specific EKMA Calculations of 28 June 1976.....	53
8	Comparison of Ozone Predictions for Four Different Models on 28 June 1976 and 24 August 1976 in Sacramento.....	55
9	Values for Maximum Ozone Versus Values for Initial Conditions.....	59
10	Control-Strategy Comparisons for San Francisco between LIRAQ and EKMA Applications.....	70
11	Initial Conditions Used in the Level III EKMA Calculations for 26 July 1973 in the San Francisco Region.....	75

32R/1

12 Sensitivity of Control-Strategy Evaluation to HC/NO_x Ratio for Trajectory 1--26 July 1973..... 79

13 Sensitivity of Control-Strategy Evaluation to Trajectory Path..... 83

14 Control-Strategy Comparisons Using a New-Style Isopleth.... 85

15 SAI Airshed Model Predicted Peak Ozone Concentrations Computed for Different Control Strategies in the Hypothetical Region 89

16 Emission Rates and Mixing Heights Used in EKMA Applications to Hypothetical Region Control Strategies..... 91

17 Trajectory Model Outputs Used as Inputs for the EKMA Simulations..... 92

18 Comparison of Maximum Predicted Ozone for the SAI Airshed, SAI Trajectory, OZIPM/CBM, and City-Specific EKMA Models: Base-Case Conditions Used for the Control-Strategies Study of the Hypothetical Region..... 93

19 Control-Strategy Study Total Emissions Resulting from a 30 Percent Reduction in Mobile HC and NO_x Emissions..... 96

20 Comparison of Maximum Ozone Predictions between the Trajectory Model, OZIPM/CBM, and City-Specific EKMA with Different Control Scenarios..... 97

21 Initial Conditions Used in the Level III EKMA Calculations for Hypothetical Region for 24 August 1976 Meteorology 98

EXHIBITS

1 Q-tapes and Q-files Provided to the EPA by the BAAQMD..... 10

32R/1

1 INTRODUCTION

The Environmental Protection Agency (EPA) has developed a method for estimating the emission controls that will be needed to meet the National Ambient Air Quality Standard (NAAQS) for ozone (O_3) concentrations in urban areas. This method, known as the Empirical Kinetic Modeling Approach (EKMA), uses an isopleth diagram for ozone concentrations that is related to hydrocarbon (HC) and nitrogen oxide (NO_x) precursor levels. Each point on the isopleth diagram represents the maximum one-hour ozone level reached as a result of the specific HC and NO_x combination described by the abscissa and ordinate values of the isopleth diagram. The ozone value generated from each HC and NO_x combination is obtained by a computer-based trajectory model--OZIPP (Whitten and Hogo, 1978a). OZIPP contains many simplifying assumptions that are designed to strike a balance between factors such as the state of knowledge, data availability, computer size, predictive accuracy, and overall cost.

This report presents the results of one of several studies that evaluate the EKMA. The approach taken in this particular evaluation of the EKMA uses gridded input files that were previously prepared for use with large, sophisticated airshed models of the grid variety. One of these models--LIRAQ--was used to prepare an Air Quality Maintenance Plan (AQMP) for the San Francisco urban area (BAAQMD, 1979). The other--the SAI Urban Airshed Model--had been used in a mobile-source-control evaluation study conducted for the California Department of Transportation (DOT) (Reynolds et al., 1979) in the Sacramento region. When the gridded data from these more sophisticated models are input to the OZIPP trajectory model, the results can be compared with those of the other models to form one basis for evaluating the EKMA.

This study also compared the OZIPP trajectory simulations either with observed data or with predictions made by the other models on the basis of change in emissions values. In addition, parts of this study involved alternative input assumptions and changes to the model definitions so that both sensitive parameters and improvements to the EKMA could be evaluated.

1.1 Background and Objectives

For several years the Office of Research and Development of the EPA has sponsored a coordinated program consisting of fundamental chemical research, smog chamber experimentation, and model development. The objective of this program is to develop mathematical models capable of simulating the dynamics of the chemical reactions and dispersion of the gaseous pollutants found in the lower troposphere. These atmospheric models are to be used both to gain an understanding of air pollution and to predict the probable outcome of control scenarios. To this end, the EPA Office of Air Quality Planning and Standards (OAQPS) has embarked on an extensive program of model comparison and evaluation.

The specific purpose of the OAQPS program is to assess the suitability of available photochemical oxidant modeling approaches for use by states as planning tools in ozone air quality planning and management. The program includes comparisons and evaluations of the various approaches for typical U.S. cities. As part of the program, large, detailed data bases are being assembled for several example cities.

The primary objective of this study is to evaluate one such approach--the EKMA--through the application of the photochemical trajectory model that forms its basis. This model is used to generate isopleth diagrams of constant urban ozone maximums as a function of the morning precursor levels of nonmethane hydrocarbons (NMHC) and nitrogen oxides. The EKMA method uses these results to estimate, in a relative manner, the precursor control requirements necessary to reduce ozone levels below the National Ambient Air Quality Standard for ozone. The method was developed for use at several levels of sophistication, depending on the extent of input data available. If the basic model is fundamentally sound, the simulated results should approach the observed values as the availability of detailed data increases.

The EPA has prepared highly detailed data concerning precursor emissions, meteorology, and ambient air quality for Tulsa and Philadelphia to test various air quality simulation models such as the OZIPP and the SAI Urban Airshed Model. In addition, there are data bases already available for St. Louis, Los Angeles, San Francisco, and Sacramento. Because some models are grid-based and thus designed to reproduce spatial and temporal variations within the metropolitan airshed, detailed information files are required. The availability of detailed data and of the results from parallel studies using sophisticated models offers the following advantages for making an in-depth study of the EKMA:

> The simple application of the OZIPP trajectory model, using either the actual available data inputs or the

corresponding data simulated in other models, should generate results that can be compared both with ambient air data and with the results of the other models. The timing of results regarding data such as the ozone maximums and precursor decay should also be comparable.

> Tests of the sensitivity of the results to variations in the input data can demonstrate important data requirements for successful application of OZIPP. This information should be useful in determining cost effectiveness for future uses. The results of the sensitivity study are also useful for improving the trajectory model in case the present version does not adequately simulate observed ambient data or the simulations of more complex models.

> The application of the EKMA procedures to air quality planning demonstrates the utility of the EKMA compared with that of methods based either on simpler models (such as a rollback model) or on more complex models (such as the SAI Urban Airshed Model).

> The potential effectiveness of OZIPP model improvements can be assessed using the results of the complex models as a standard.

2 SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

2.1 SUMMARY

We have evaluated the EKMA by comparing OZIPP with other models previously applied to the San Francisco and Sacramento regions. The study was carried out at several levels, beginning with the trajectory model that forms the basis of the EKMA and ending with the control-strategy predictions that result from employing the EKMA methodology. In the San Francisco region OZIPP was compared with the LIRAQ model, which was used for the 1979 Air Quality Maintenance Plan (AQMP). In the Sacramento region comparisons were made with the SAI Airshed Model, which has been applied in a study for the Department of Transportation (Reynolds et al., 1979).

The basic OZIPP model is a simple, moving-air-parcel, or trajectory, model that uses a detailed chemical mechanism for the surrogate propylene and butane hydrocarbons. Time-dependent, precursor-emissions factors can be treated, along with expansion of the air parcel, and entrainment is treated by assuming that constant concentrations exist outside the parcel.

2.2 CONCLUSIONS

The primary emphasis of this comparison study was directed toward the discovery of features in the trajectory model that could explain differences in the results of OZIPP from those of some other model. To that end, most of the OZIPP simulations utilized initial conditions derived from the model used for comparison purposes. Thus, for the most part, the study used the LIRAQ and Airshed Model data files to generate appropriate OZIPP inputs. Although the utilization of these files tends to circumvent the issue of normal-source data preparation, the comparison of models is clarified by use of common data bases. Furthermore, costs are minimized. For some of the OZIPP simulations, we used air quality data rather than information common to the comparison model. This step allowed the categorization of overall differences as either effects resulting from the data utilized or those attributable to specific features of the models.

This study, and a similar study by Whitten and Hogo (1981) using Los Angeles data, show that OZIPP can provide results that are often quite similar to those of the more complex models. By carefully separating the models according to specific formulation differences and through careful analysis of intermediate results, the most important feature in formulation that produced different results between two models could often be isolated. Even though the absolute values predicted by the OZIPP trajectory model may be significantly different from those of the more complex models (one of the main differences is often a result of the different chemical mechanisms employed), the isopleth applications of the EKMA (which uses the trajectory model results in a relative fashion) typically show control predictions corresponding to those of the more complex models.

In the comparison of the EKMA results with those of the LIRAQ model for the San Francisco region, primary attention was given to the trajectory leading to the design ozone of the AQMP. Although there are uncertainties associated with deriving any specific trajectory path, in this study the air parcel that eventually affects the site of maximum ozone concentration (Livermore) apparently originates at 0800 PDT over the Pacific Ocean just south of San Francisco. This trajectory is discussed in detail in section 3.2. It was found that the precursor loading for this trajectory and for several others was extremely sensitive to wind speed because of widely varying emissions density in the area.

Another sensitive input was the size of the air parcel. The emissions files used in the LIRAQ studies were for 5-km grids. Using a narrow size (<5 km) for the width of the EKMA trajectory made the results sensitive to the exact choice of a path between, or over, the grid squares of the LIRAQ inventory. Sometimes the emissions density changed by more than two orders of magnitude between adjacent grid squares. For most cases, a 10-km width produced reasonable and similar results for slightly different trajectory paths. Some trajectories were 15 km wide, roughly coinciding with the size of the city of San Francisco proper, the main source of the emissions.

The SAI Airshed, or grid, Model served as the basis of the Sacramento study. SAI trajectory model simulations were made using recreated input files from the earlier grid model study. In some instances, important differences between grid and trajectory model results could not be resolved. For these cases, the study focused largely on comparing the OZIPP results with those of the SAI trajectory model (rather than the grid model) because the trajectory model was used to generate input data for OZIPP. Obtaining data directly from the trajectory model eliminated many uncertainties in the model comparisons, such as those related to model size, wind speed, or mixing depths. Differences due to model formulation

thus became more apparent than those of the LIRAQ comparisons. The most sensitive differences, both absolutely and relatively, were found in the chemical mechanisms.

The SAI models used in the Sacramento study employed an early version of the Carbon-Bond Mechanism (CBM) (Whitten, Hogo, and Killus, 1980). In general, the CBM chemistry generated higher absolute levels of ozone than the standard EKMA chemistry. In the control-prediction phase, the two chemistries predicted similar results when HC and NO_x were simultaneously reduced; but the CBM chemistry predicted more ozone reduction than the standard EKMA chemistry when HC reductions only were involved. Although the OZIPP model and the SAI trajectory model are much different in terms of complexity (apart from chemistry), these factors apparently did not play a significant role for the Sacramento area. Thus, such factors as multilevel mixing, eddy diffusion, elevated emissions, and variable concentrations aloft were found to be unimportant when common input data were used.

2.3 RECOMMENDATIONS

The following considerations are suggested for future studies:

> For cases in which differences in control-strategy predictions are found to be related to differences in the chemistry employed in various models, it is important to investigate the chemical reactions that produce these differences. If appropriate smog chamber experiments that would validate one or the other types of mechanisms can be identified, these experiments should be performed.

> A generic concept can be associated with the EKMA that goes beyond its present formulation and uses. Developmental work on the EKMA should continue to update its formulation and improve its utility. Specifically, the following steps are suggested:

- This study demonstrates that significant differences in both absolute model results and in predicted control requirements can sometimes occur when the Carbon-Bond Mechanism is substituted for the propylene/butane chemistry currently used in OZIPP. Further studies should be undertaken to investigate and resolve potential discrepancies between the two mechanisms.

- Credibility of the EKMA could be enhanced by providing a means for considering urban hydrocarbon reactivity. Either the latter should be related to the propylene reactivity used in OZIPP, or the chemical mechanism utilized in the OZIPP should be changed to be compatible with available reactivity information.

- Isopleths based on emissions inventories might be further developed to perhaps replace the present initial-condition-based isopleths. Urban HC and NO_x measurements are often not relevant to the initial conditions that are appropriate to a city-specific trajectory, as this study demonstrated for several of the San Francisco trajectories.

- The mixing-depth algorithm should be improved so that the changes with time correspond to observations rather than produce a constant-dilution factor.

- The transported pollutants, both in the surface layer and aloft, might be varied according to the level of control of emissions. The variance could be controllable by the user. The current procedure necessitates two separate isopleth diagrams. (Again, further development would be necessary to incorporate this refinement.)

- The regular city-specific algorithm might be modified to allow optional starting times in place of the present 0800 PDT starting time. Earlier starting times would emphasize dependence on an emissions inventory, whereas later starting times might emphasize dependence on initial conditions.

> Modifications to the current version of the EKMA have also been suggested in other studies. Although such suggestions have not been addressed in this study, their implementation might also be considered.

- The two-stage approach (in which stationary-source emissions are held constant in the first stage and mobile-source emissions are held constant in the second stage) might be further developed so that local districts can use EKMA isopleths to make the control predictions for stationary emissions.

- Point-source emissions might be handled so that the interaction with all possible urban HC/NO_x concentrations could be evaluated as part of a new source review procedure.

- Percent cutback diagrams (PCD) might be added to the OZIPP code so that both the isopleth and the PCD are generated.

- Temperature changes, deposition, variable reactivities, nitrate chemistry, and sulfate chemistry can also be added to OZIPP. Isopleths of species other than ozone can also be generated by OZIPP.

- Statistical packages can be combined with the EKMA to generate the probable number of exceedances resulting from various control scenarios.

> The use of more complex models such as the SAI Airshed Model should be accompanied by the use of the EKMA, both for absolute trajectory simulations along the path to the major ozone peaks and for control-strategy guidance from the isopleth diagrams. The studies performed to date show that unless the wind fields are complicated by such factors as wind shear, the two types of models normally give similar results. In the absence of complex meteorological factors, important differences in results would indicate the existence of problems in one or both of the models that should be investigated.

3 TRAJECTORY MODEL APPLICATIONS

This section focuses on applying an EKMA-type trajectory model to predict absolute values of ozone. Predictions were made for several cases in San Francisco and Sacramento. The predicted ozone levels were compared with observed concentrations, when these were available, and with predictions of more complex models. The results can be used to assess the fundamentals of the formulation model and to identify important differences between models.

3.1 San Francisco Applications

The 1979 air quality maintenance plan for the Bay Area Air Quality Management District (BAAQMD) was developed using the Livermore Regional Air Quality (LIRAQ) Model (BAAQMD, 1979). During this study, sufficient air quality, emissions, and meteorological data were collected to permit application of the OZIPP-type trajectory model. The trajectory model predictions could then be compared with both observed data and the LIRAQ predictions. Furthermore, the control strategies tested using the LIRAQ model could be tested using the EKMA technique to compare its utility with that of the more complex LIRAQ model. (The control strategy tests are addressed in greater detail in chapter 5.)

The LIRAQ model was used to simulate the distribution of photochemical pollutants in the BAAQMD on two days--26 July and 20 August 1973. The data necessary for applying the LIRAQ model on these two days are available on tapes supplied by the BAAQMD and are identified in exhibit 1. Many of these data have also been reported by Feldstein et al. (1979) and others. Using the data for these two days, we undertook specific case studies using the OZIPP-type trajectory model. Case studies for one additional day (24 July 1974) were also performed, even though the results could not be compared with those of the LIRAQ model, but only with observed air quality data.

In the discussion that follows, the LIRAQ model and the OZIPP-type trajectory model are first described. Then, specific case studies are discussed. Finally, the overall results are summarized.

Attention:
John Summerhays (MD-14)

SHIPPING LIST

Q-TAPES AND Q-FILES PROVIDED TO EPA, PLR BAAQMD-ABAG CONTRACT

BAAQMD Assigned Q-Tape Number	File Number	Description of Q-Files, in Order on Q-Tape
1	1	QSRUN, July 26, 1973
	2	QSOR, 1975 Baseline, Region 1, 5 Kms
	3	QICON, July 26, 1973
	4	QGEO
	5	QRAD, July 26, 1973
		Nota Bene; GEO repeated on Q-Tape 9, QSOR for 75 Baseline, Region 1, 5 Kms, is repeated on Q-Tape 7.
2	1	QTRANO, July 26, 1973
	2	QTRAN1, July 26, 1973
	3	QTRAN2, July 26, 1973
	4	QTRAN3, July 26, 1973
3	1	QICON, Nov 5-6, 1976
	2	QTRANO, Nov 5-6, 1976
	3	QTRAN1, Nov 5-6, 1976
	4	QTRAN2, Nov 5-6, 1976
	5	QTRAN3, Nov 5-6, 1976
4	1	QICON, July 24, 1974
	2	QTRANO, July 24, 1974
	3	QTRAN1, July 24, 1974
	4	QTRAN2, July 24, 1974
	5	QTRAN3, July 24, 1974
5	1	QSOR, 2000 Baseline, Region 1, 5 Kms
	2	POP, 2000 Baseline, Region 1, 5 Kms
	3	AIR, 2000 Baseline, Region 1, 5 Kms
	4	CAR, 2000 Baseline, Region 1, 5 Kms
	5	PNT, 2000 Baseline, Region 1, 5 Kms
	6	SKY, 2000 Baseline, Region 1, 5 Kms
6	1	QSOR, 1985 Baseline, Region 1, 5 Kms
	2	POP, 1985 Baseline, Region 1, 5 Kms
	3	AIR, 1985 Baseline, Region 1, 5 Kms
	4	CAR, 1985 Baseline, Region 1, 5 Kms
	5	PNT, 1985 Baseline, Region 1, 5 Kms
	6	SKY, 1985 Baseline, Region 1, 5 Kms
7	1	QSOR, 1975 Baseline, Region 1, 5 Kms
	2	POP, 1975 Baseline, Region 1, 5 Kms
	3	AIR, 1975 Baseline, Region 1, 5 Kms
	4	CAR, 1975 Baseline, Region 1, 5 Kms
	5	PNT, 1975 Baseline, Region 1, 5 Kms
	6	SKY, 1975 Baseline, Region 1, 5 Kms
8	1	QMRUN, July 24, 1974
	2	QMET, July 24, 1974
	3	QMRUN, Nov 5-6, 1976
	4	QMET, Nov 5-6, 1976
		Nota Bene; These are all MASCON inputs.
9	1	QGEO
	2	QMRUN, Aug 20, 1973
	3	QMET, Aug 20, 1973
	4	QMRUN, July 26, 1973
	5	QMET, July 26, 1973
		Nota Bene; These are all MASCON inputs. QGEO repeated on Q-Tape 1. QGEOs identical.
10	1	QSRUN, Aug 20, 1973
	2	QICON, Aug 20, 1973
	3	QTRANO, Aug 20, 1973
	4	QTRAN1, Aug 20, 1973
	5	QTRAN2, Aug 20, 1973

EXHIBIT 1. Q-TAPES AND Q-FILES PROVIDED TO THE EPA BY THE BAAQMD

3.1.1 Model Definition

The LIRAQ model is of the grid variety, providing estimates of pollutant concentrations as a function of time throughout the modeling region. The model mathematically simulates the complex physical and chemical interactions taking place in the atmosphere, employing a lumped parameter chemical mechanism to describe the photochemical reactions taking place. Specifically, the model predicts instantaneous pollutant concentrations in single-layer grids superimposed on the modeling region. Surface concentrations are estimated by an analytic function. For a more detailed description of the model, the reader is referred to the study of MacCracken and Sauter (1975).

The intent of applying the OZIPP-type trajectory model is to follow the evolution of photochemical pollutants, particularly ozone, along the air parcel trajectory leading to an observed, peak ozone concentration. This approach is consistent with that which the EPA has termed a Level II analysis (Federal Register, 1979). The standard EKMA trajectory model contained in the computer program OZIPP (Whitten and Hogo, 1978a) was not applicable to such an analysis; however, the subsequent program OZIPM (Whitten and Hogo, 1978b), contains options that facilitate such applications and, thus, was used in this study.

The OZIPP model was based on the reactions of high initial precursor concentrations in a major urban-source region. The model follows the original air parcel throughout the day as it travels to a suburban site where ozone maximums have been observed. This conceptual pattern was similar to the pattern of ozone development seen in the smog chamber experiments used to validate the OZIPP model (Dimitriades 1977; Dodge, 1977). The OZIPM model permits the use of alternative starting times and hourly mixing height inputs that are more representative of the conditions considered in this study. This version of the model also provides the option of replacing the standard EKMA chemistry with other mechanisms. As described later, this option was used in some portions of the study.

The detailed trajectory model approach using the OZIPM model requires the definition of numerous variables, including the air parcel trajectory leading to a peak ozone level; initial pollutant concentrations within the air parcel; the diurnal variation in mixing height; emissions occurring along the trajectory path; pollutant concentrations above the mixed layer that may later be entrained into the surface-based mixed layer; and chemical reactivity. The procedures for defining these variables are described in the following subsections.

3.1.1.1 Trajectory

To specify trajectories describing the leading of air parcels to elevated ozone levels, first, the two highest observed ozone concentrations for each of the three study days were obtained from the LIRAQ QICON (the file containing observed air quality data). Wind-field maps were then created using the LIRAQ QMET input files for these days. For example, on 26 July 1973, the maximum ozone level was 0.176 ppm at Livermore at 1700 PDT. According to the LIRAQ surface wind-field maps, the direction and speed for the previous hour (1600 to 1700 PDT) at Livermore was 25 km/hr at 250°. The location of the air parcel at 1600 PDT was thus determined by moving 25 km from Livermore at an angle of 250°. This procedure was repeated for each preceding hour until the parcel reached the ocean.

In this case, the trajectory ending at Livermore had passed over South San Francisco in the morning. According to the QMET file for this day, wind vectors were to the north and south of the trajectory. The peninsula to the south of San Francisco is a source of high emissions and the composition of the air parcel is thus extremely sensitive to the speed with which it travels across the peninsula. Because the trajectory passed directly over the San Francisco International Airport (SFO), wind speed data from the airport were used with the QMET data to determine the trajectory path across the peninsula.

By definition, then, the trajectory path ended at a point of high ozone concentration. However, additional concentration values also were available from the closest monitoring station for the hour during which the trajectory passed by. The contour lines presented in the LIRAQ reports (see MacCracken and Sauter, 1975) show that, at least, the ozone levels simulated in the LIRAQ model do not have many steep gradients. Therefore, the nearest station value and LIRAQ model predictions could also be compared to the OZIPM predictions along the trajectory path.

3.1.1.2 Initial Concentrations

All trajectory paths studied for the San Francisco area appeared to originate over the Pacific Ocean. Thus, initial concentrations were considered to be insignificant and, therefore, were assumed to be at background levels. Sensitivity of model predictions to this assumption is further evaluated in chapter 4.

3.1.1.3 Mixing Heights

Mixing heights were obtained from the LIRAQ QTRAN files. Since these data are presented for three-hour periods only, values for the remaining hours were obtained by linear interpolation. Thus, a mixing height for 0800 PDT would be two-thirds of the 0700 PDT value plus one-third of the 1000 PDT value. The mixing heights used in this study are given in table 1.

The mixing layer typically increases in thickness as the warm surface air erodes the inversion layer. Under such conditions air is entrained from aloft that, in turn, increases the volume of the conceptual air parcel of the OZIPM trajectory model. Under some circumstances the change in mixing height may not be a result of entrainment from aloft. For instance, an air mass moving at high velocity would initially tend to flow over a stagnant air mass. Also, in areas of convergent wind flow such as in the case of air passing from open terrain into a canyon, mixing height can be pushed up from the sides. In this type of change in mixing height--narrowing of the sides of an air parcel, accompanied by an increase in the height of the air parcel--the volume of the air parcel may not change. Since changes in the mixing height in the OZIPM model are intended to represent a change in volume for the moving air parcel, changes in mixing height that do not reflect a change in volume should not be included as input data. Unfortunately, the wind flow in complex terrain is not easily separated into mixing-height changes, either those accompanied by entrainment of air from the sides or those accompanied by entrainment of air from aloft. Although entrainment of air into the sides of the EKMA model could be treated as entrainment from aloft, the basic concepts behind the OZIPM model suggest that such air is considered to contain concentrations identical with those of the model parcel itself. Therefore, the data related to air entrained from the sides would normally be ignored along with any changes in volume associated with such phenomena.

3.1.1.4 Emissions

The version of OZIPP that is available in the OZIPM computer code contains options for post-0800 emissions of both HC and NO_x. For virtually all the trajectories used in this study, initial conditions were not significant, and the emissions occurring along the trajectory were responsible for the ozone maximums. The OZIPM model uses post-initial emissions input data in the form of fractions related to the initial concentrations. If the initial HC concentration was 1 ppm, emissions during some subsequent hour sufficient to add an additional 1 ppmC would merely be included in OZIPM as 1.0 for that hour. If the inversion height

TABLE 1. INPUT DATA FOR THE SAN FRANCISCO TRAJECTORIES

(a) Initial Concentrations

Species	Transported Pollutants Surface	Aloft
NO_x	0.001	0.01
NMOC	0.01	0.05
O_3	0.0	0.04

NO_2/NO_x = 0.5.
Surface hydrocarbon reactivity: standard OZIPP conditions.
Aloft hydrocarbon reactivity: standard OZIPP conditions.

(b) Emission Hydrocarbon Reactivities

	26 July 1973		20 August 1973		24 July 1974	
Species	Trajectory 1	Trajectory 2	Trajectory 1	Trajectory 2	Trajectory 1	Trajectory 2
PROP	0.221	0.203	0.223	0.275	0.226	0.225
BUT	0.779	0.797	0.777	0.725	0.774	0.773
FORM	0.008	0.007	0.007	0.008	0.008	0.008
ACET	0.012	0.011	0.011	0.012	0.012	0.013

(c) Mixing Height
(m)

Date	Morning Mixing Height PDT	Afternoon Mixing Height PDT
26 July 1973--trajectory 1	100 at 0800	137 at 1300
26 July 1973--trajectory 2	60 at 0800	750 at 1700
20 August 1973--trajectory 1	204 at 0800	730 at 1500
20 August 1973--trajectory 2	142 at 0800	410 at 1600
24 July 1974--trajectory 1	50 at 0800	250 at 1700
24 July 1974--trajectory 2	50 at 0800	670 at 1600

32R/14

TABLE 1 (Continued)

(d) Emissions

26 July 1973--Trajectory 1

Time (PDT)	NOx (ppm)	HC (ppmC)
1000	0.019	0.172
1100	0.043	0.457
1200	0.001	0.198
1300	0.037	0.491
1400	0.0001	0.006
1500	0.0007	0.046
1600	0.0015	0.042
1700	0.0038	0.034

26 July 1973--Trajectory 2

Time (PDT)	NO_x (ppm)	HC (ppmC)
1300	0.0028	0.0481
1400	0.0594	0.8337
1500	0.0597	0.7324
1600	0.0241	0.2483
1700	0.0214	0.336

20 August 1973--Trajectory 1

Time (PDT)	NO_x (ppm)	HC (ppmC)
0700	0.0089	0.0546
0800	0.0262	0.2304
0900	0.0002	0.0490
1000	0.0080	0.1223
1100	0.0103	0.0569
1200	0.0056	0.0494
1300	0.0038	0.1575
1400	0.0038	0.1559
1500	0.0042	0.0628

TABLE 1 (Concluded)

20 August 1973--Trajectory 2

Time (PDT)	NO_x (ppm)	HC (ppmC)
1100	0.0159	0.1849
1200	0.0002	0.0007
1300	0.0052	0.0002
1400	0.0219	0.0041
1500	0.0001	0.0001
1600	0.0086	0.0011
1700	0.0524	0.0032

24 July 1974--Trajectory 1

Time (PDT)	NO_x (ppm)	HC (ppmC)
1200	0.0055	0.1452
1300	0.0919	0.960
1400	0.0712	1.402
1500	0.0400	0.4207
1600	0.0233	0.1145
1700	0.0150	0.1283

24 July 1974--Trajectory 2

Time (PDT)	NO_x (ppm)	HC (ppmC)
1000	0.0079	0.139
1100	0.0828	0.859
1200	0.0207	0.180
1300	0.0268	0.200
1400	0.0123	0.252
1500	0.0183	0.372
1600	0.0627	0.694
1700	0.0591	0.479

changed between the time of the initial condition and the time of subsequent emissions, the computer code would automatically adjust the emissions factor.

The LIRAQ QSOR input file for 1975 was used to determine the source emissions. The data in this file, expressed in units of gm/sec/grid-cell, with 5-km grid cells, were converted to ppm using the following information:

$$\frac{\text{moles}}{\text{liter}} = \underset{\substack{\uparrow \\ \text{value in QSOR file}}}{\frac{\text{grams}}{\text{sec-grid cell}}} \cdot \underset{\substack{\uparrow \\ \text{M W}}}{\frac{\text{mole}}{\text{gram}}} \cdot \underset{\substack{\uparrow \\ \text{one hour to second conversion}}}{\frac{3600 \text{ sec}}{\text{hr}}} \cdot \underset{\substack{\uparrow \\ \text{inversion height in meters}}}{\frac{\frac{1}{z}}{}} \cdot \underset{\substack{\uparrow \\ \text{convert to liters}}}{\frac{1}{1000 \text{ } \ell/\text{m}^3}} ,$$

$$\text{ppm} = \frac{\text{moles}}{\text{liter}} \cdot \underset{\substack{\uparrow \\ \text{ideal gas}}}{\frac{24.4 \text{ } \ell}{\text{mole}}} \cdot 10^6 .$$

The LIRAQ emissions inventory was prepared by dividing all emissions of hydrocarbons into three categories (propylene, butane, and aldehydes) for use in the LIRAQ chemical mechanism (see MacCracken and Sauter, 1975). Therefore, the alkane and alkene values were multiplied by 4 (i.e., butane) and 3 (i.e., propylene), respectively, to obtain units in ppmC. The alkane, alkene, and aldehyde values were added for each hour to obtain the hourly hydrocarbon emissions. The reactivities used are given in table 1.

The width of the trajectory was determined by the emissions gradient. In one case, there was as much as a factor of 100 between grid cells, and a 15-km-wide trajectory was used.

3.1.1.5 Pollutant Concentrations Aloft

Aircraft data (see MacCracken and Sauter, 1975, pp. 871-948) were used to determine the concentrations aloft. The values used were the average of the measured quantities obtained when the aircraft was above the OZIPM trajectory. Because hydrocarbon data for 1977 were not available, data for 1974 were used. The concentrations used are given in table 1.

3.1.1.6 Chemistry

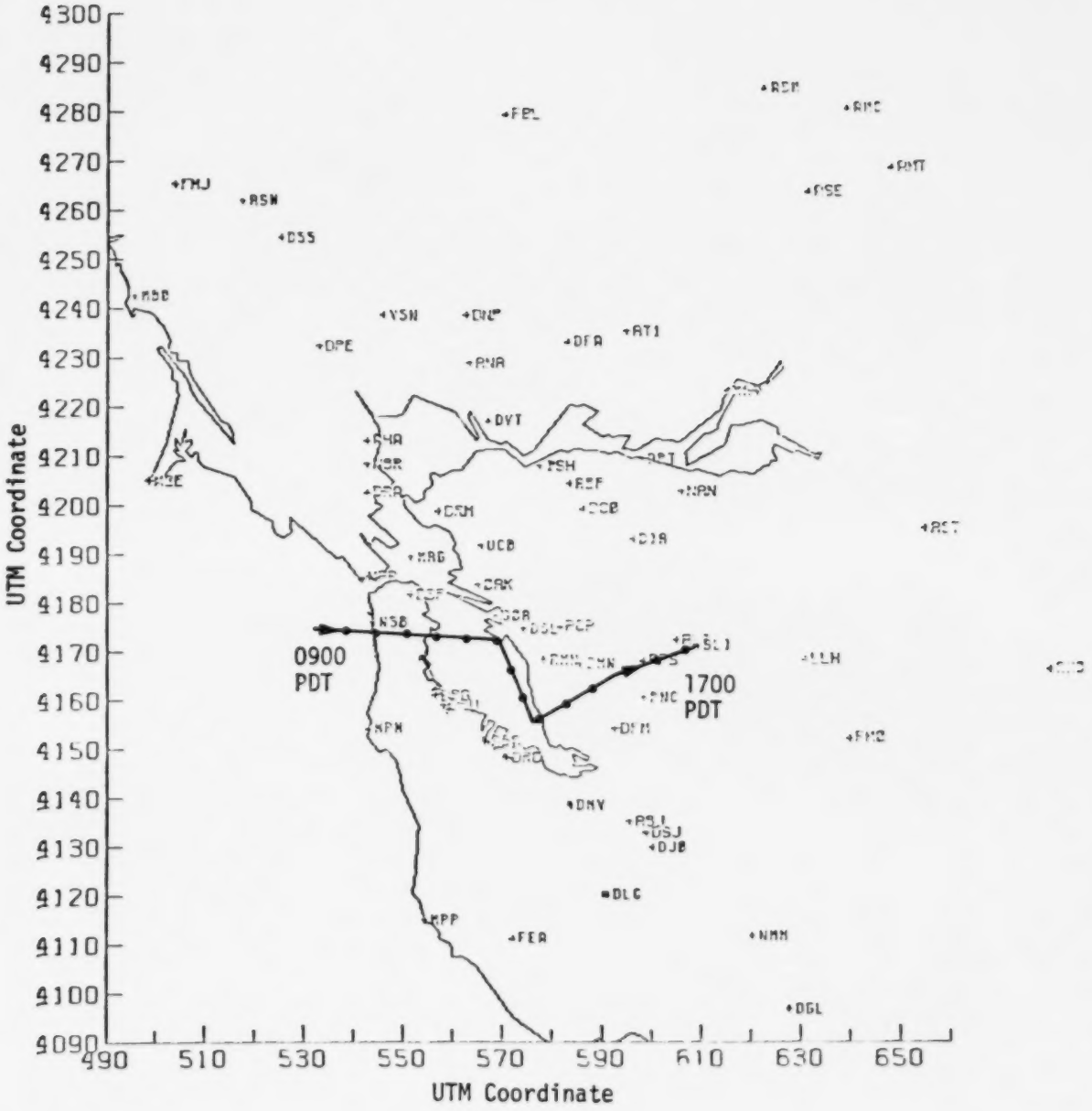
In all cases, the standard EKMA chemistry was employed, but the reactivity and aldehyde fractions were taken from the LIRAQ input files. The effects of considering a different chemical mechanism for evaluating a control strategy are addressed in chapter 5.

3.1.2 San Francisco Case Studies

The six trajectories developed for the San Francisco region are illustrated in figures 1(a) through 6(a). In each case the final destination was chosen to coincide with a monitoring station. Figures 1(b) through 6(b) illustrate the results of the six trajectory model runs for this region. The HC emission profiles used in the OZIPM computer code are also shown, along with observed ozone values and those computed by the LIRAQ model.

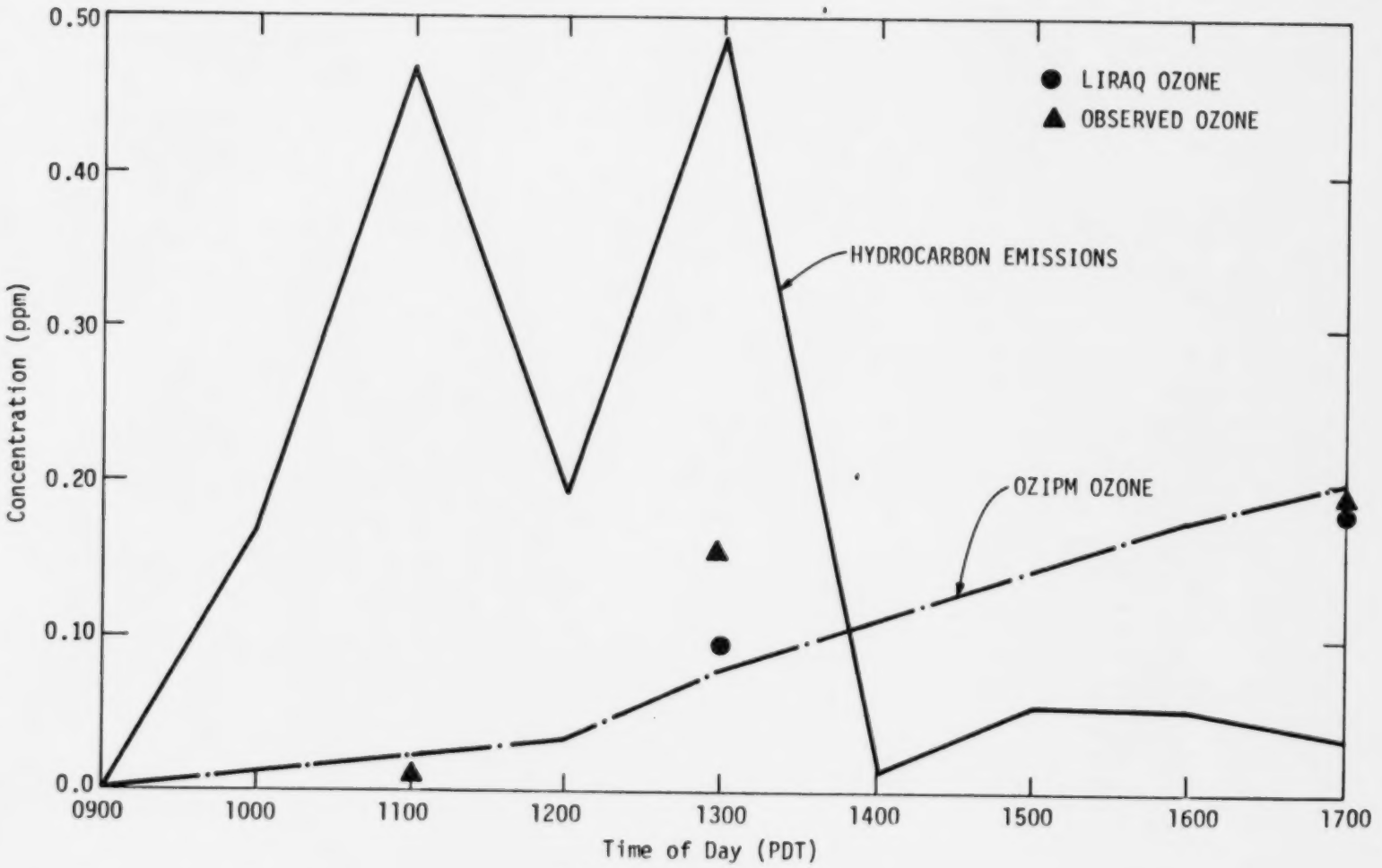
The main emphasis in this study was applied to the 26 July 1973 trajectory shown in figure 1. This trajectory was chosen because it represented the trajectory to the highest observed ozone concentration for the prototype meteorology day modeled in the LIRAQ study. According to our analysis of available wind data, the air parcel that eventually affects the Livermore area originates at 0800 PDT over the ocean just south of the city of San Francisco. Between 0900 and about 1000 hours, the trajectory passes over the San Francisco peninsula where emissions from four major freeways and San Francisco International Airport are added to the emissions from the industrial area of South San Francisco. The air parcel then passes over the bay and veers south along the east shore where freeways and industrial emissions from the Oakland area are entrained and, finally, moves east through a canyon into the Livermore Valley. As documented in chapter 4, the model results are extremely sensitive to wind speed because of the precursor emissions injected along the trajectory.

The simulation results for trajectory 2, 26 July 1973, are shown in figure 2. There is a dip in the simulated ozone profile at 1600 PDT because of a large and sudden increase in mixing height (163 to 700 m in one hour). One complication in comparing LIRAQ and the OZIPM stems from the analytical function used in the LIRAQ model to simulate vertical gradients in concentration. Evidently, the analytic function used in the LIRAQ model to account for vertical mixing allows the simulated ground concentrations to respond more slowly to rapid changes in the mixing depth than is the case in the OZIPM model, which assumes instantaneous mixing throughout the mixed layer.



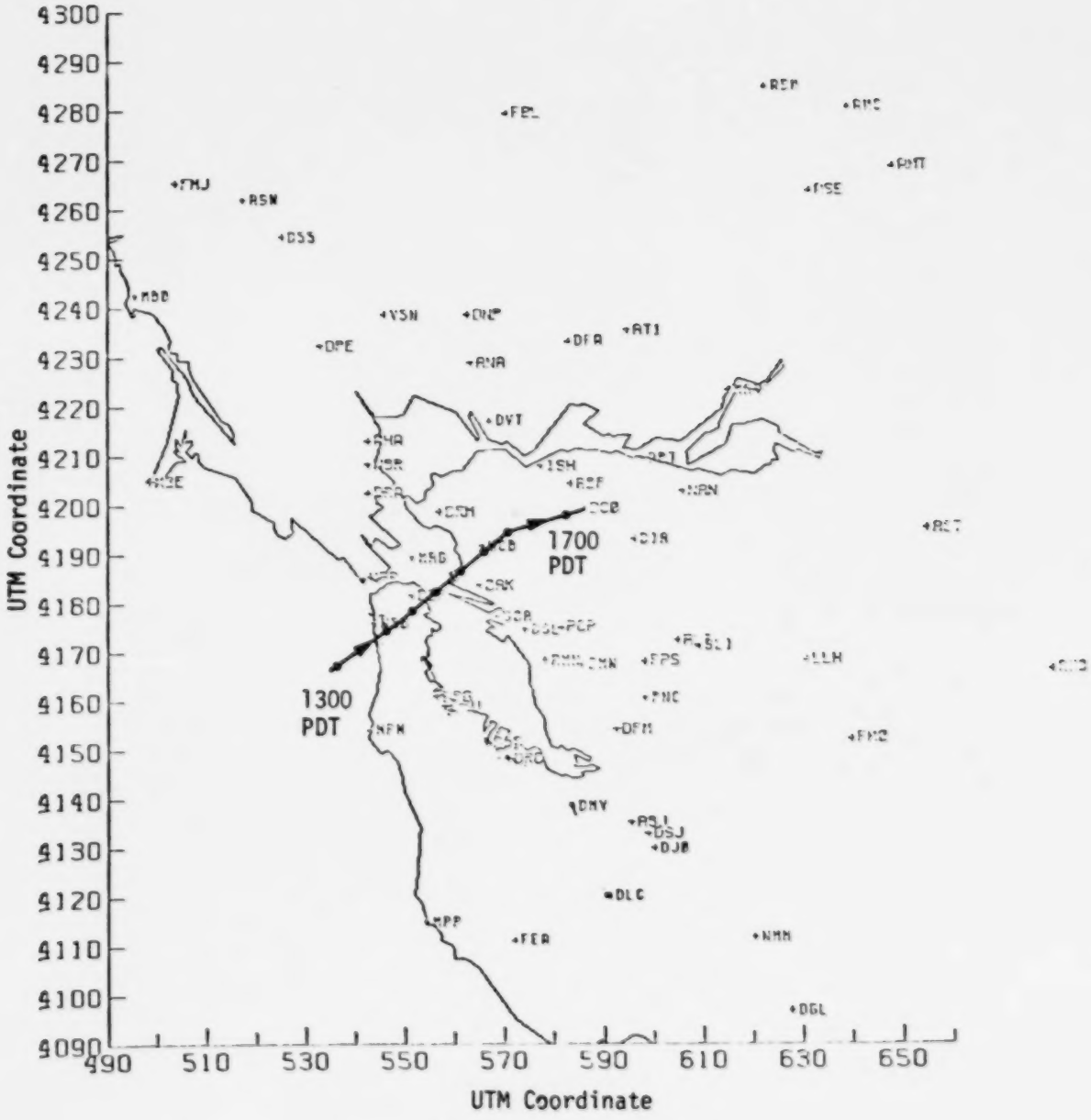
(a) Trajectory Path

FIGURE 1. TRAJECTORY 1 FOR 26 JULY 1973



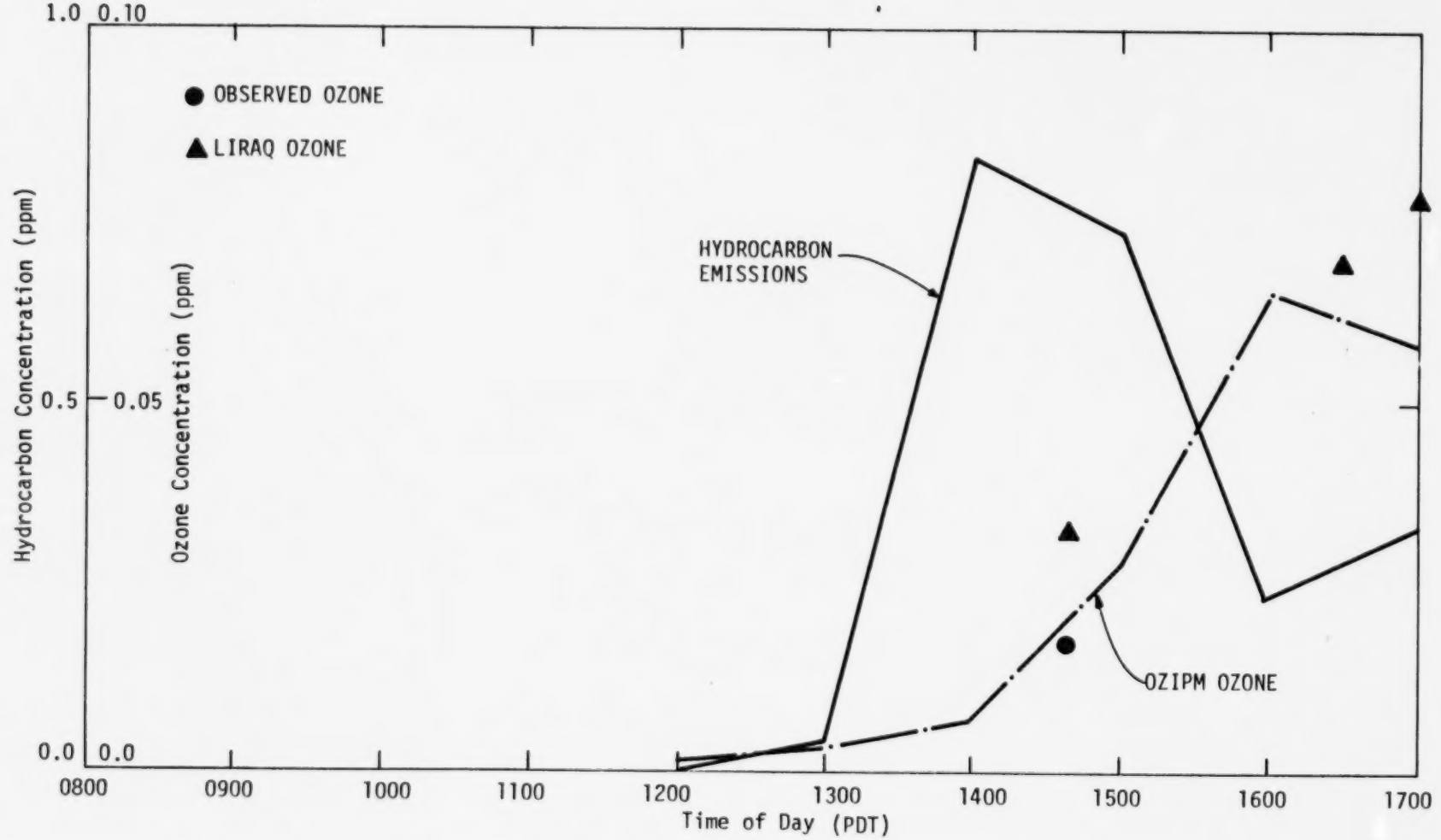
(b) Simulation Results

FIGURE 1 (Concluded)



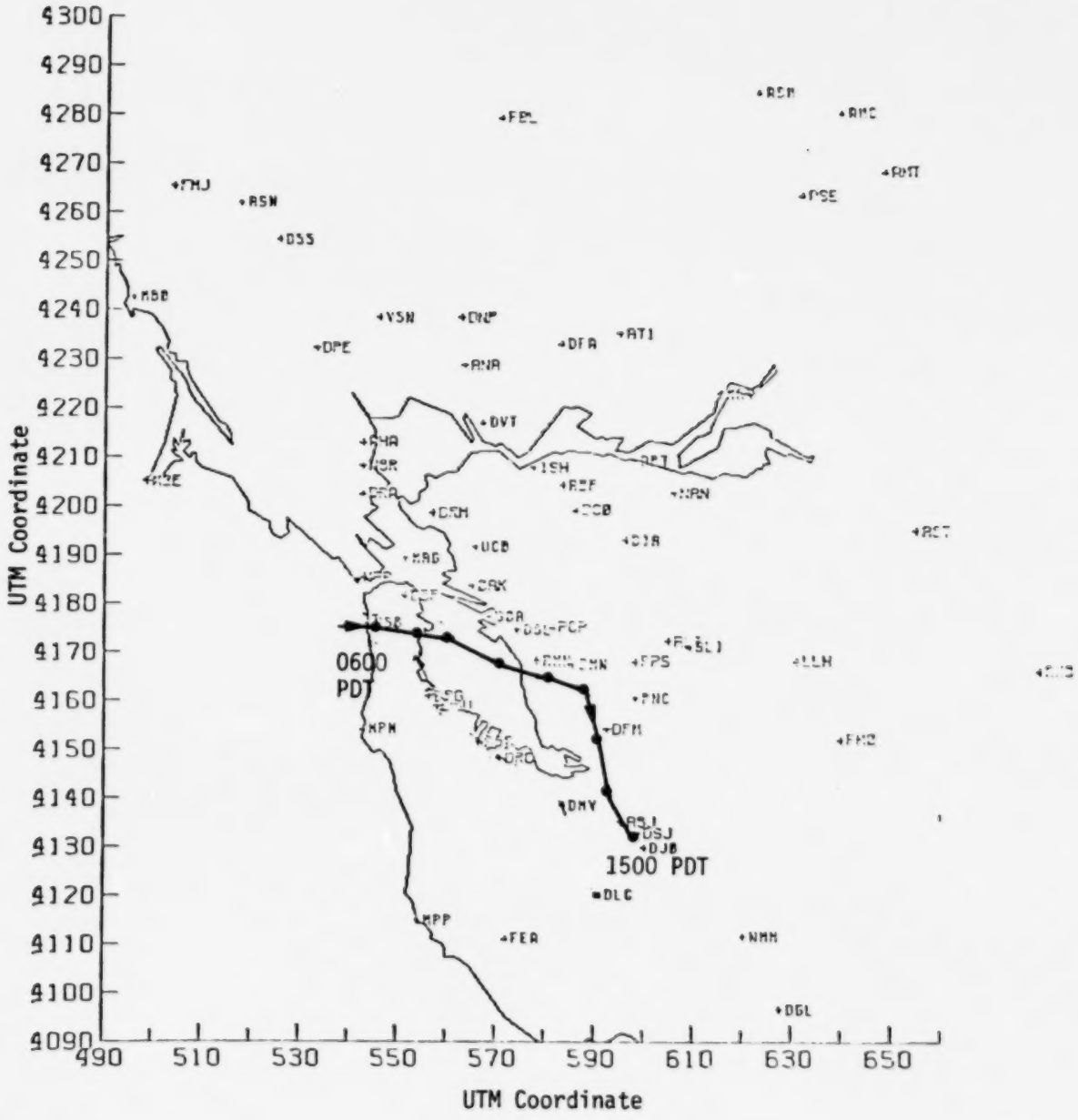
(a) Trajectory Path

FIGURE 2. TRAJECTORY 2 FOR 26 JULY 1973



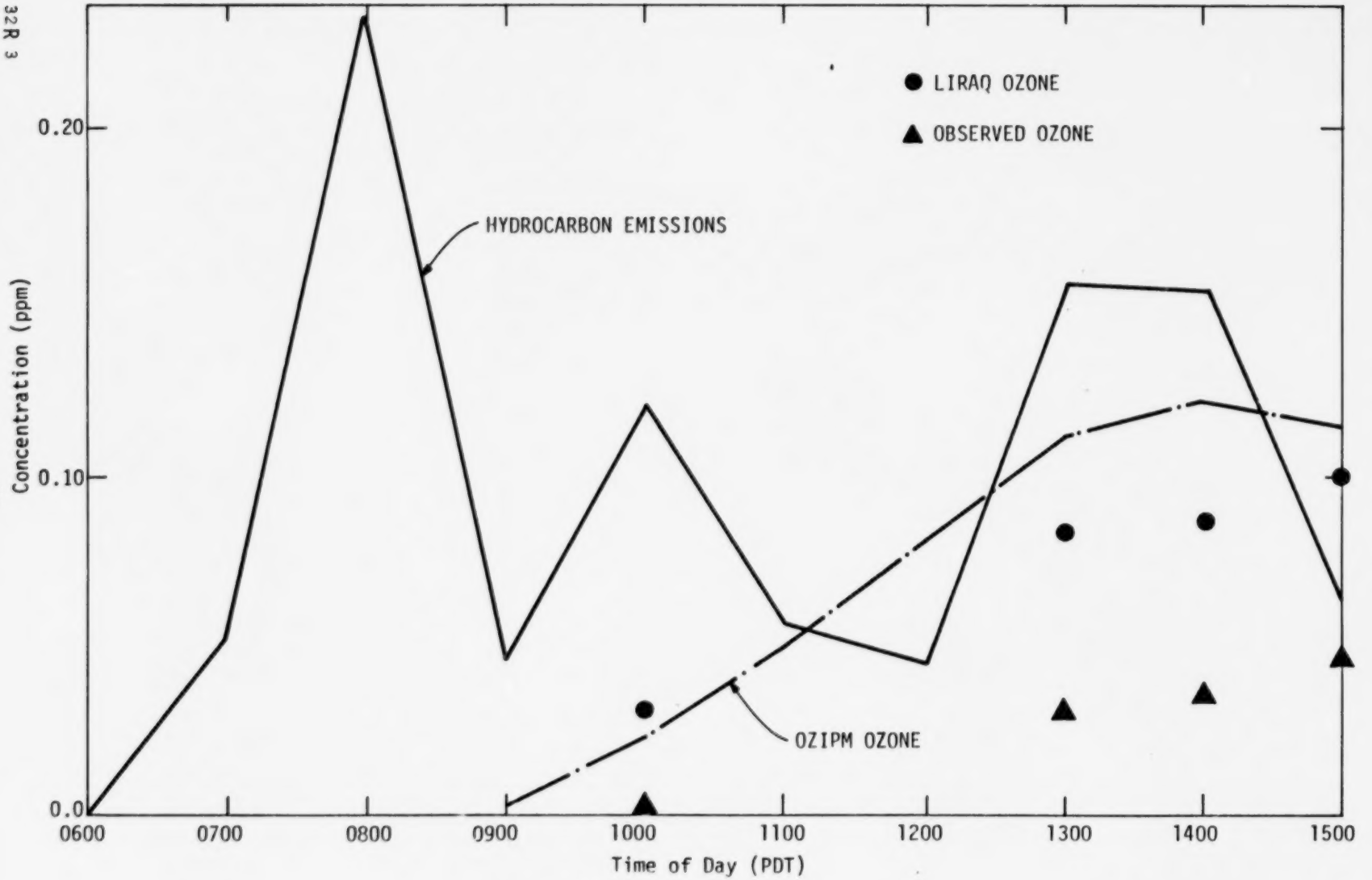
(b) Simulation Results

FIGURE 2 (Concluded)



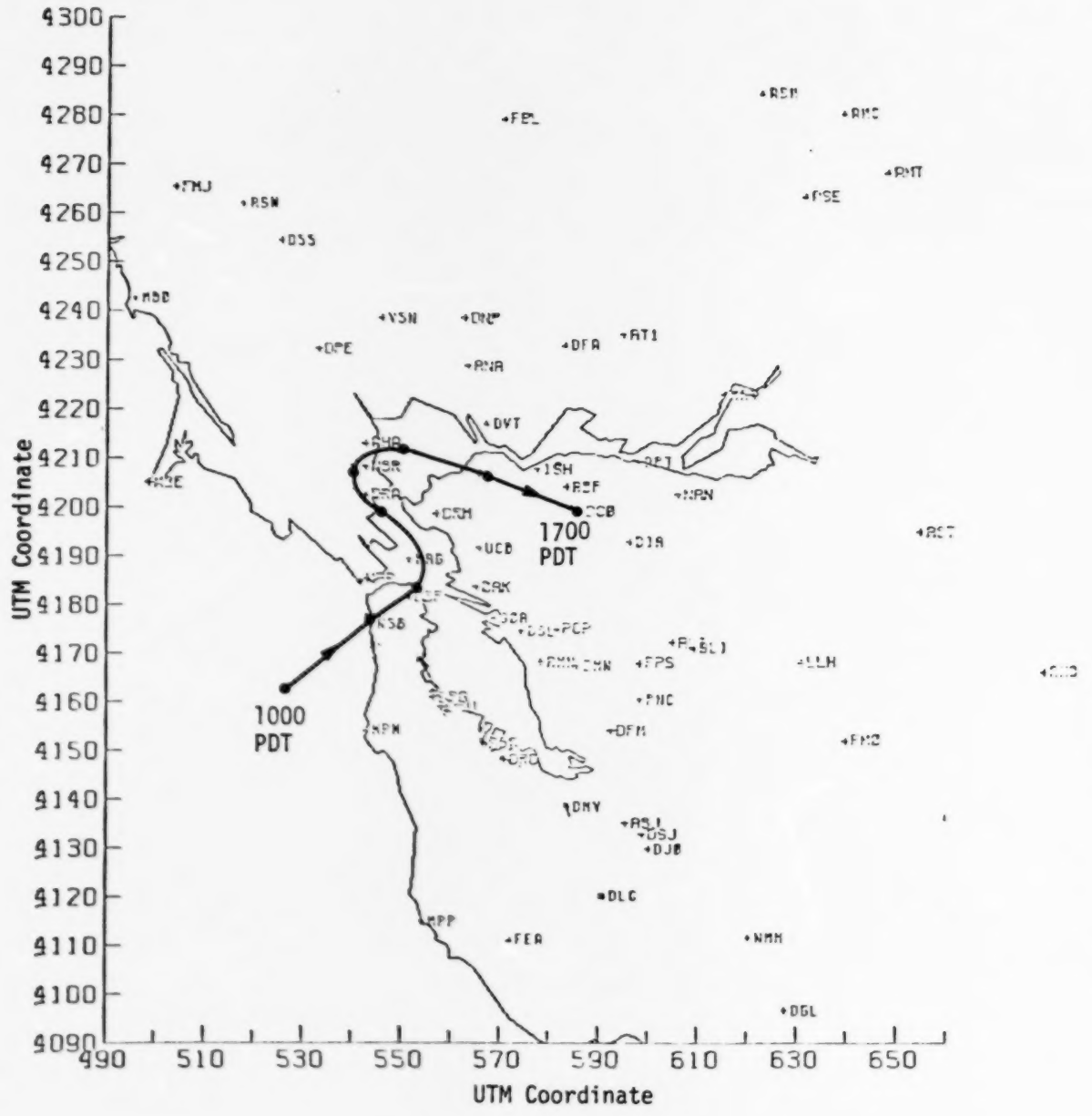
(a) Trajectory Path

FIGURE 3. TRAJECTORY 1 FOR 20 AUGUST 1973



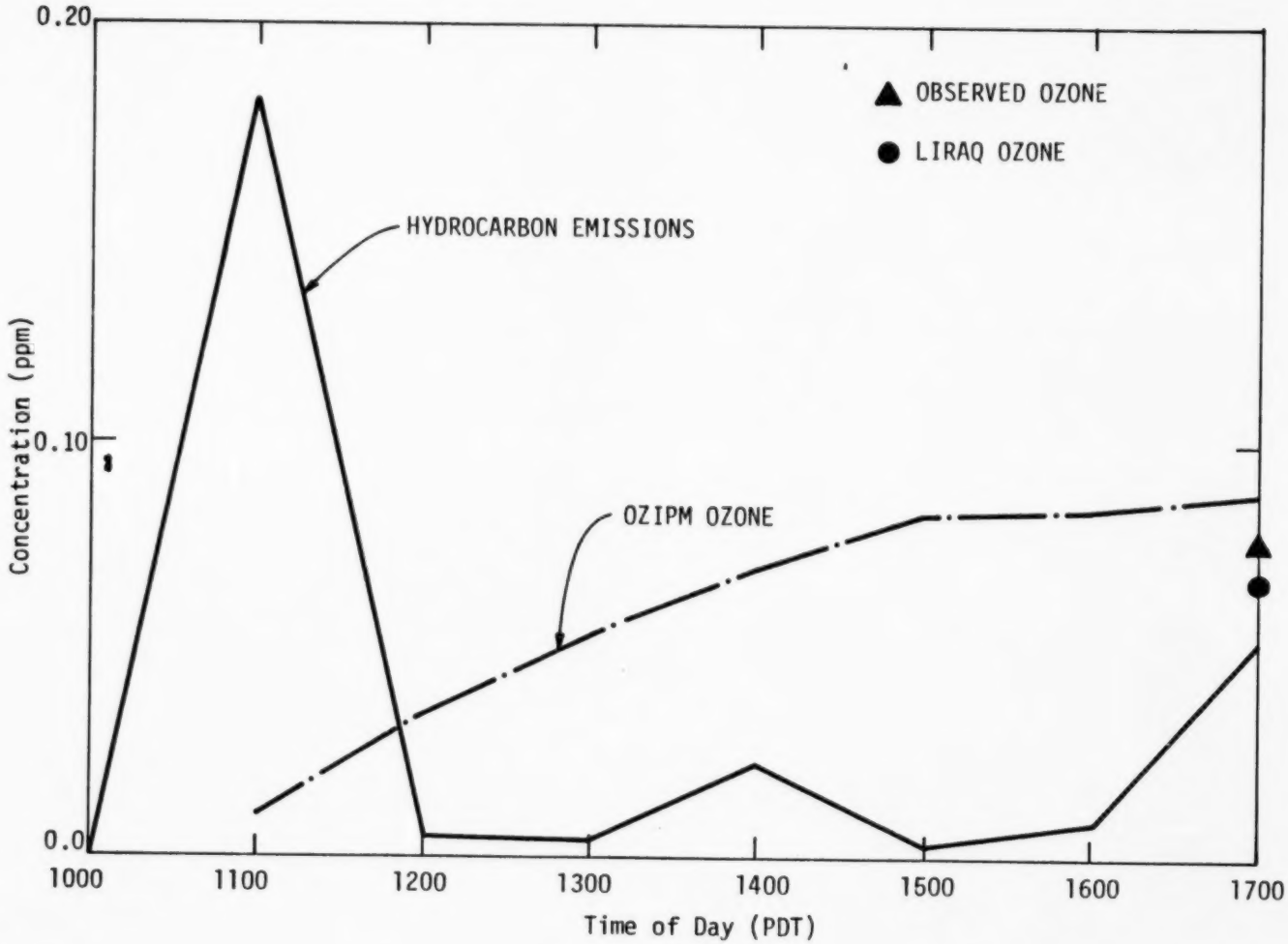
(b) Simulation Results

FIGURE 3 (Concluded)



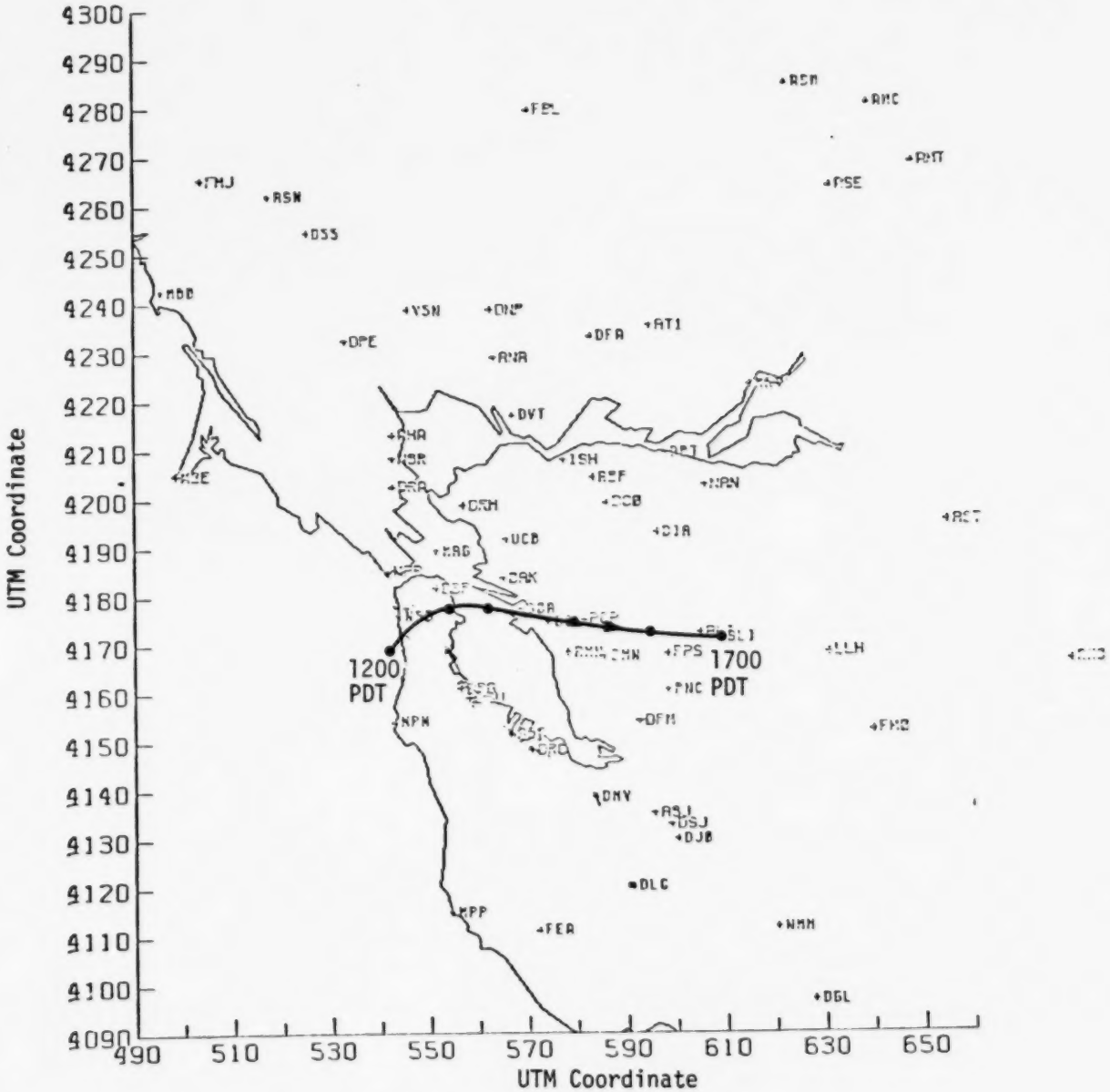
(a) Trajectory Path

FIGURE 4. TRAJECTORY 2 FOR 20 AUGUST 1973



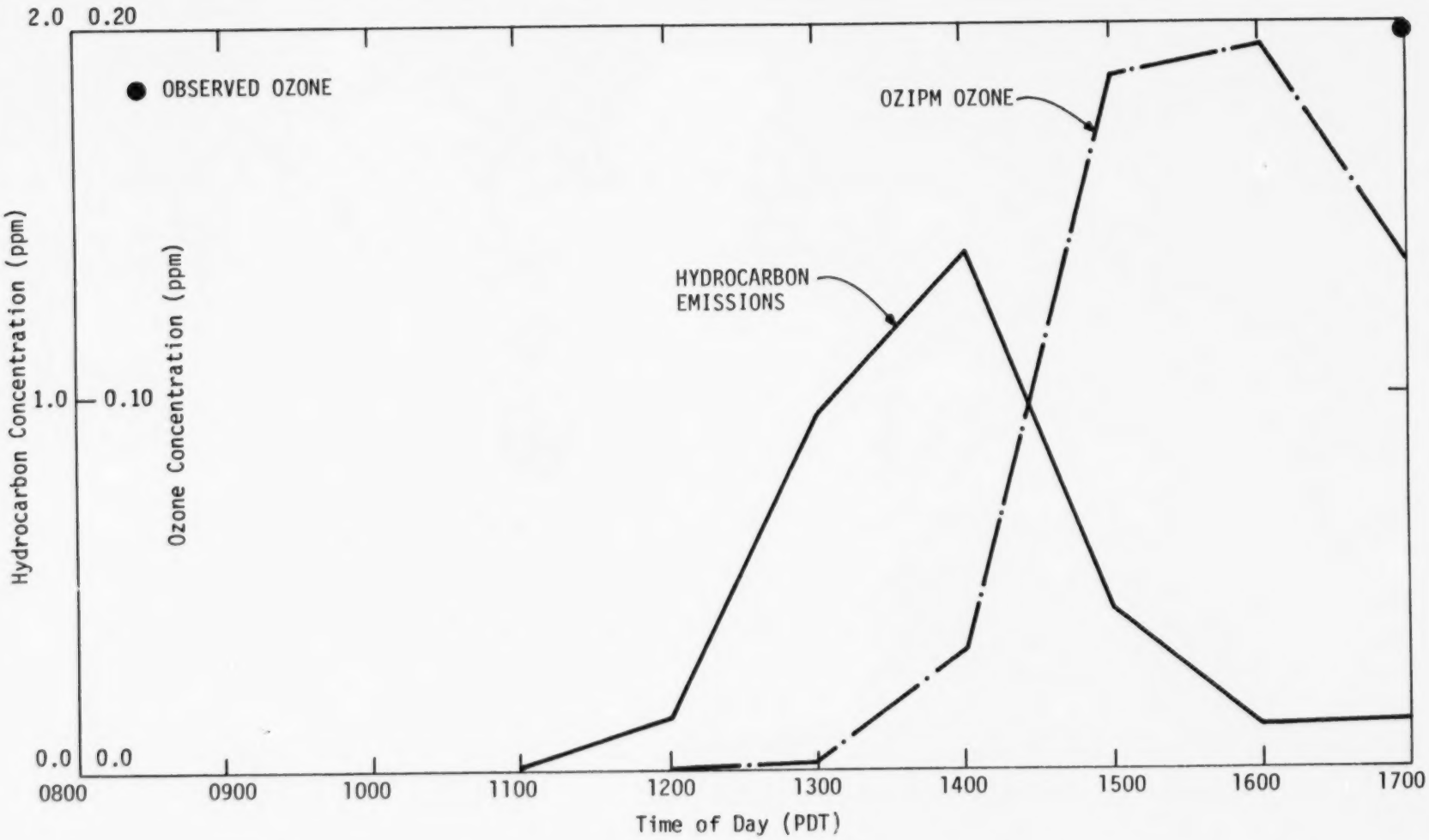
(b) Simulation Results

FIGURE 4 (Concluded)



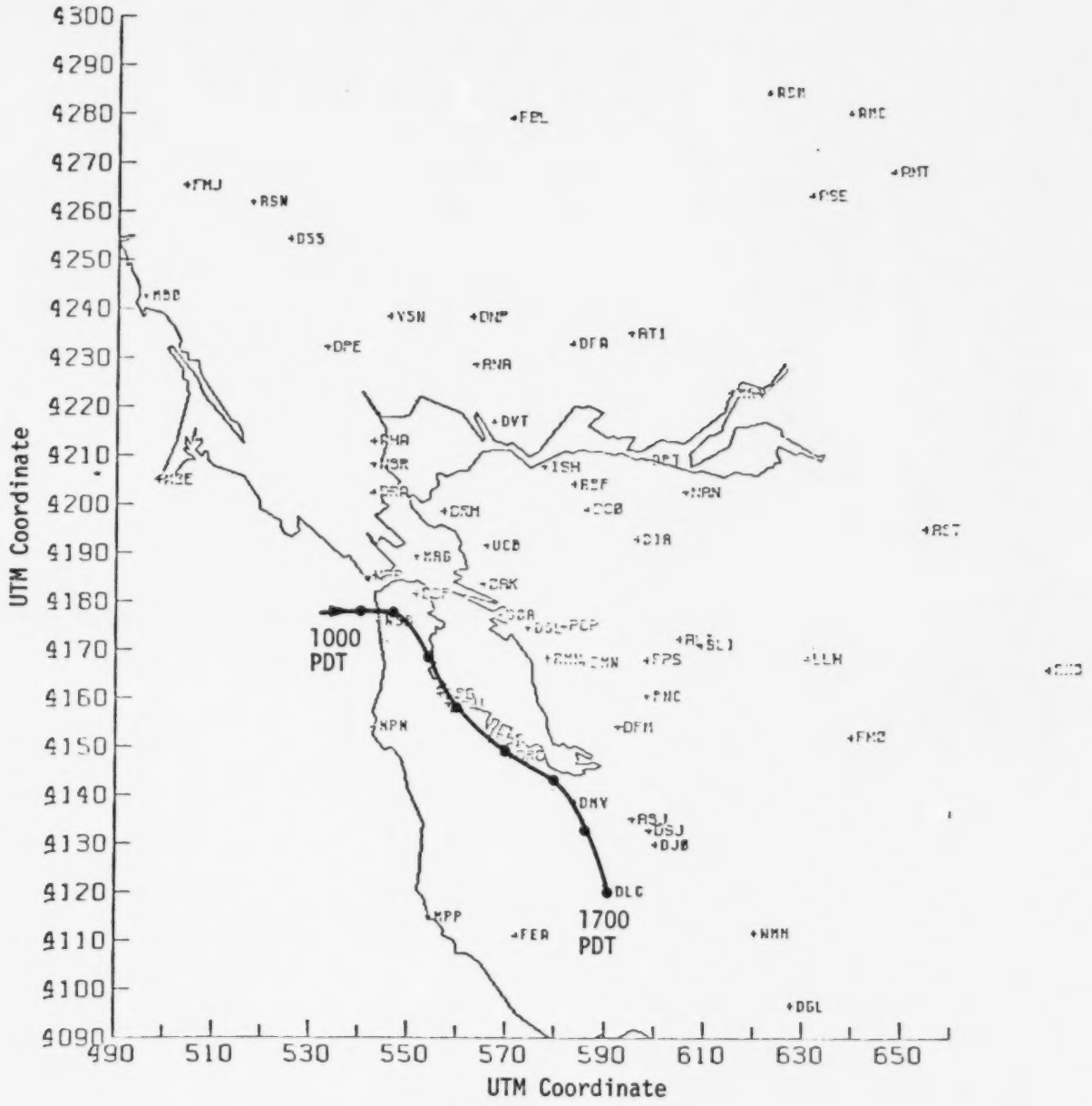
(a) Trajectory Path

FIGURE 5. TRAJECTORY 1 FOR 24 JULY 1974



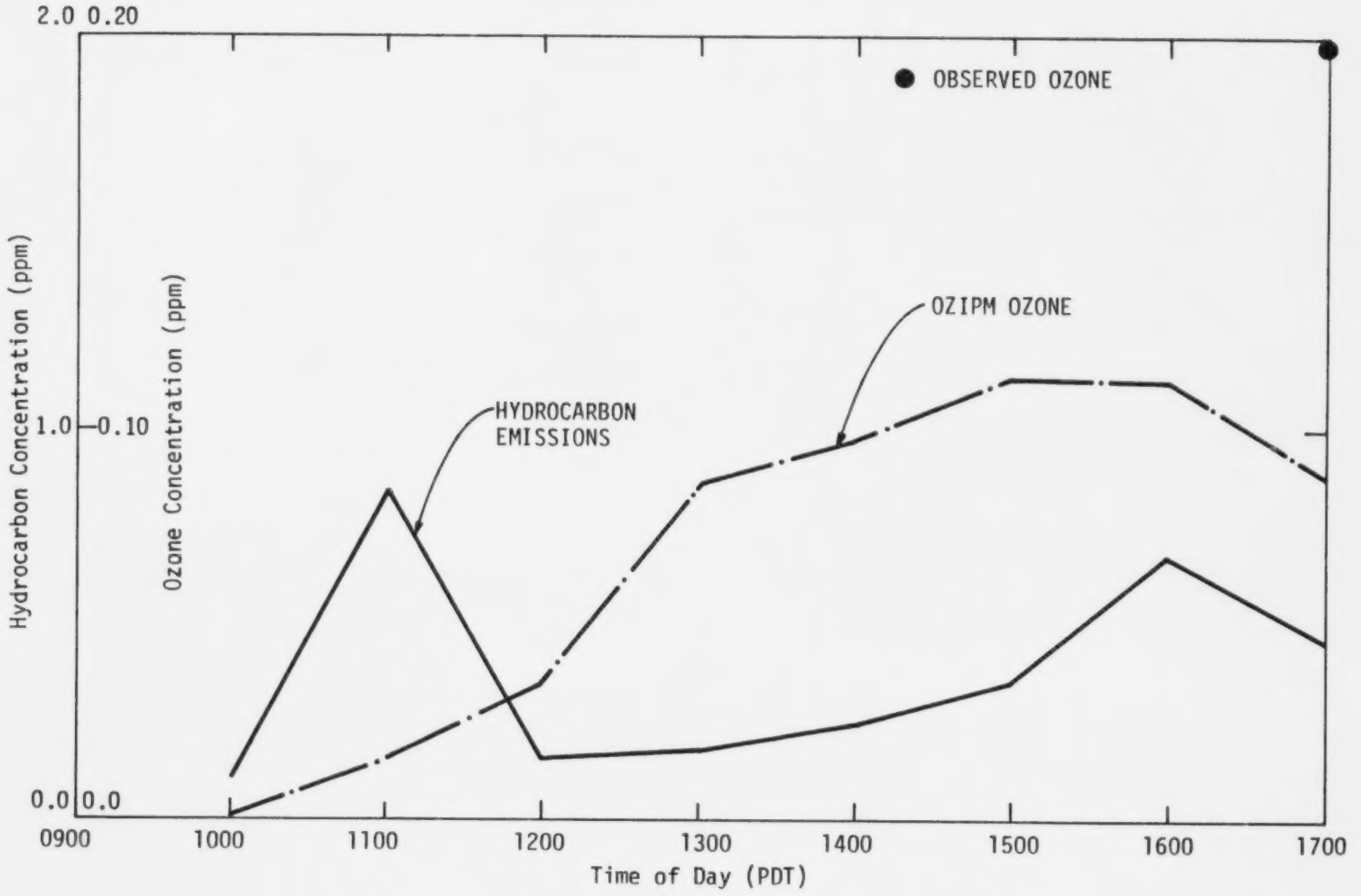
(b) Simulation Results

FIGURE 5 (Concluded)



(a) Trajectory Path

FIGURE 6. TRAJECTORY 2 FOR 24 JULY 1974



(b) Simulation Results

FIGURE 6 (Concluded)

The simulation results for trajectory 1, 20 August 1973, are shown in figure 3 and are similar to the results for the 26 July 1973 trajectory shown in figure 1 in that the injection of precursors is strongly dependent on the choice of wind speed. The sparseness of wind-speed data in the LIRAQ files and the difficulty of accurately interpreting the LIRAQ wind fields introduce large uncertainties as to the path and timing of the trajectory. The sensitivity to wind speed is discussed in section 4.

The results for trajectory 2, 20 August 1973, shown in figure 4, demonstrate a close agreement between the LIRAQ and OZIPM models and the observed ozone profile.

The trajectories of 24 July 1974, which are shown in figures 5 and 6, cannot be compared for the LIRAQ and OZIPM models because the results of the former are not available. The trajectory illustrated in figure 5 shows a drop in the ozone at 1600 PDT due to a sudden increase in the mixing height (96 to 242 m in one hour, as is the case for trajectory 2 of 26 July 1973). The most important change, which would increase the simulated ozone for the trajectory results shown in figure 6, would be a path slightly more to the west than the one shown. The emissions density on either side of the OZIPM model is quite different from that of the trajectory path, because the path determined from the LIRAQ wind fields follows the edge of the bay. This type of "path" sensitivity is also demonstrated in section 4 for the 26 July 1973 trajectory shown in figure 1.

3.1.3 Summary of Results for San Francisco Case Studies

Table 2 summarizes the results of the case studies just described. The series of six trajectories for the San Francisco region represents a severe test for a simple type of model such as that employed in OZIPM. Special care was required in using the options built into the model because of the terrain features, wind patterns, and varied emissions densities found and because of the lack of dependence on initial conditions. As discussed later in chapter 4, several factors were involved in preparing the input data, which also required careful analysis. Nevertheless, the input data selected appear to provide a reasonable level of success when the OZIPM results are compared with either observed data or the LIRAQ results.

Primary attention was given to trajectory 1 of 26 July 1973; thus, the poor results obtained for trajectory 2 of 24 July 1974 might be partially due to the failure to consider refinements to the obviously sensitive input data. However, the lack of a LIRAQ simulation for that day eliminated a principal standard of comparison and, therefore, our efforts were concentrated elsewhere.

TABLE 2. SUMMARY OF RESULTS FOR THE SAN FRANCISCO CASE STUDIES

Date	Trajectory No.	Maximum O_3 (ppm) Observed	OZIPM-Predicted	LIRAQ-Predicted
26 July 1973	1	0.18	0.20	0.19
	2		0.06	0.08
20 August 1973	1	0.10	0.12	0.04
	2	0.08	0.09	0.07
24 July 1974	1	0.20	0.19	NA*
	2	0.20	0.12	NA*

* NA = not applicable

When examining the results shown in table 1, it should be noted that instantaneous values are given for the models, but an hourly average value is given for the observed data. However, as noted earlier and illustrated in the trajectory model results shown in the figures, ozone tends to vary rather slowly near the peaks. The results shown in the figures should also be compared for timing effects. For instance, figure 5(b) shows that the OZIPM-simulated ozone peak occurs an hour before the observed peak. The terrain near the peak could involve some convergent wind flow, which would raise the mixing height without diluting it; thus, the mixing height used in OZIPM for that time (1600 to 1700 hours) might have been inappropriate. This trajectory does, in fact, follow a path similar to that of the 26 July 1973 trajectory 1 path discussed earlier. The results presented in figure 6(b) for trajectory 2 of 24 July 1974 also show that the timing and peak value might be much closer to that of the observed ozone level if convergent flow effects had been involved during the previous two hours. However, again, this possibility was not pursued.

3.2 SACRAMENTO APPLICATIONS

Air quality modeling of the Sacramento region was performed using a sophisticated three-dimensional grid model (the SAI Airshed Model) as described by Reynolds et al. (1979). In that study two 1976 ozone-episode days were modeled (28 June and 24 August). Detailed descriptions of the inputs to the Airshed Model were presented in that study. In this study, we compared the results of Reynolds et al. with the OZIPM/CBM trajectory model results and those of the regular city-specific OZIPP.

Figure 7 shows the Sacramento modeling region and the available monitoring stations. The modeling region is 50 km on each side and is divided into a 625-grid square with each grid cell 2 km on a side. The modeling region consists of four vertical levels. The first three levels are kept within the mixed layer until around noon.

In this study, we compared the results of Reynolds et al. with those of a series of less complex models. If we arrange these models on the basis of model complexity,* with a high degree of commonality among the models, comparisons of results between adjacent models can be made in a way that minimizes the number of model differences involved. A similarity in the results of adjacent models would indicate that for the particular case studied, the differences in complexity were not important.

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* By model complexity we mean the spatial and temporal detail with which the modeling is executed and also the detail with which the physical and chemical processes are represented.

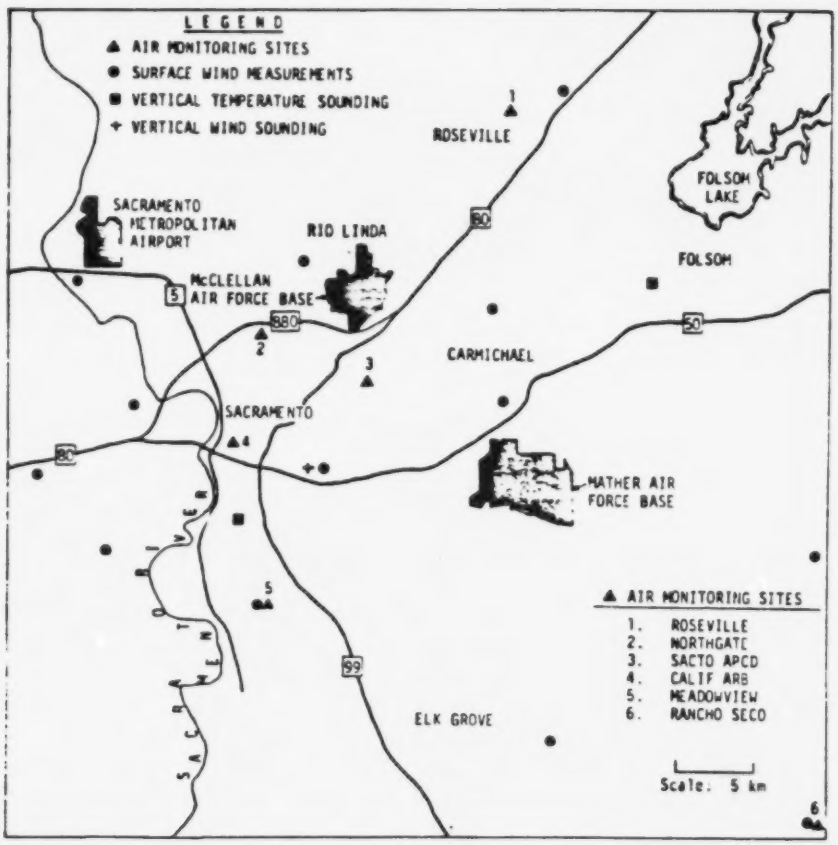

FIGURE 7. LOCATIONS OF MONITORING SITES IN THE SACRAMENTO AREA

Correspondingly, a large difference in results would apparently indicate that the features uniquely addressed by the more complex model were significant for that case.

The discussion that follows first describes the models that were applied and highlights important differences between them. Details are then presented for two case studies performed for the Sacramento area. The final section of this chapter summarizes the results of these studies.

3.2.1 Model Definition

The following list briefly describes the series of four models used in this study. They are described in greater detail in the discussions that compare them. Some models are distinguished only by the mode of application.

> The SAI Urban Airshed Model. This model is similar in concept to the LIRAQ model applied to San Francisco.

> The SAI trajectory model. In terms of inputs, computations, and results at points along a selected trajectory this model differs from the Airshed Model only through the elimination of horizontal dispersion and convergent and divergent winds.

> An EKMA-style model (OZIPM/CBM), which uses the same chemistry (Carbon-Bond) and mixing heights as the SAI trajectory model. (In this case, the model is the same as the OZIPM model described for the San Francisco study, except that the regular EKMA chemistry has been replaced with the Carbon-Bond chemistry.)

> The regular city-specific OZIPP model incorporating the standard EKMA chemistry.

In this section we wish to highlight the major differences among the models.

3.2.1.1 Comparison of the SAI Grid and Trajectory Models*

These models were designed to complement each other and, therefore, many algorithms are identical for both models (several subroutines of the computer codes are actually shared); furthermore, they use the same input files. The trajectory model begins on a square of the grid model at a specific time. The path of the trajectory is then determined solely by the wind speed and direction in the lowest level of the grid-model files. Because the other levels in the grid model often advect with velocities that are different from this lowest level, the two models often generate different results as the simulations progress in time. Nevertheless, the trajectory model provides an inexpensive method for testing parts of the grid model.

A special feature of the trajectory model is its ability to be operated backward in time. This feature was used to generate the trajectories used in this study. The time and location of either the observed or the simulated ozone maximum were used to start the backward trajectory to 0600 hours. Thus, the forward trajectories always arrived at the desired spot at the proper time for comparison with either observations or grid-model results. Changes in emissions often lead to changes in the time and location of maximum ozone concentrations. Small changes in times of maximum ozone concentration at some specific monitoring site can be associated with rather large differences in the location of the origin, and in the actual pathway taken by, the air parcel producing the specific ozone maximum. Therefore, when compared with a grid model, any trajectory model used as a tool for control strategies possesses the inherent shortcoming of being incapable of accounting for these changes.

3.2.1.2 Comparison of the SAI Trajectory Model and the OZIPM/CBM Model

The following similarities and differences exist between the trajectory model and the OZIPM/CBM developed for this comparison:

> Chemistry. Both models used in this study employ Carbon-Bond chemistry identical to that of the Airshed Model. However, the photolytic constants are computed differently in the OZIPM/CBM and SAI models. For this study, we modified the regular OZIPM/CBM values for NO_2 photolysis using a constant factor so that all models agreed at 1300 PDT. In the Airshed Model and trajectory model, the rates

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* Detailed discussions of this comparison are available elsewhere (see Reynolds et al., 1979).

of all other photolytic reactions vary with NO_2 photolysis, with a fixed ratio for each; but in the OZIPM/CBM the photolysis rates vary independently. Aldehyde photolysis was adjusted in the OZIPM/CBM to give agreement between the models at 1100 PDT.

Actually, these differences in photolysis rates constitute an advantage in sophistication for the OZIPM/CBM. The NO_2 photolysis rates normally used in the OZIPM/CBM are somewhat lower than those used in the SAI models because the latter formerly used an algorithm based on older data. Incidentally, the SAI models are now being updated to the OZIPM/CBM NO_2 photolysis rates, which are those recommended by Demerjian, Schere, and Peterson (1980). Since the purpose of the present study was to compare the OZIPM/CBM with previously computed results of the Airshed Model, we were forced to alter the OZIPM/CBM models to eliminate this difference rather than wait for the older SAI studies to be rerun with the newer photolysis rates for NO_2.

The use of fixed ratios to NO_2 photolysis in the SAI models in place of the variable ratios used in the OZIPM/CBM model may lead to some minor differences in chemistry. The ratios are at a maximum at solar noon and a minimum at sunrise and sunset (Whitten, Killus, and Hogo, 1980). The photolysis rates for aldehydes change more with solar zenith angle than the NO_2 photolysis rate does because aldehydes photolyze at the short wavelength end of the solar spectrum, whereas NO_2 photolyzes nearer the long wavelength end of the ultraviolet spectrum. The short ultraviolet wavelengths are more affected by the ozone in the stratosphere than the longer wavelengths. At high zenith angles (morning and evening), the solar rays must pass through a thicker layer of ozone. Therefore, the ratio of aldehyde photolysis to NO_2 photolysis varies throughout the day, reaching a maximum at solar noon. For this particular study, the OZIPM/CBM aldehyde photolysis values were multiplied by a constant value throughout each day so that the models agreed at 1100 PDT. Therefore, in the early morning the photolysis rate of the aldehydes in the OZIPM/CBM would be somewhat less than that used in the SAI models.

For this particular study, we chose to modify the OZIPM/-CBM to make it as much like the Airshed Model and trajectory model as possible. By removing a[illegible] possible

potential variables between models, we hoped to be able to better compare the fundamentals underlying these models. The CBM version of OZIPM/CBM has normally been applied to assist users of the Airshed Model to estimate potential control scenarios. For such applications the photolysis adjustments discussed here are normal. Perhaps for this study an additional series of tests with OZIPM/CBM using the regular EKMA photolysis rates would have been helpful, but they were not performed during that phase of this contract.

> Reactivity. The SAI trajectory model and Airshed Model are operated with reactivity splits that vary with each source category. However, the OZIPM/CBM does not have this feature; instead, reactivity is assumed to be constant for all hydrocarbon emissions throughout the day. For this study, the OZIPM computer code was modified so that three different hydrocarbon reactivities could be used: one for the initial conditions, one for the aged hydrocarbons aloft, and one for the emissions that occur throughout the day. Hence, the only differences in reactivity were in the temporal variations aloft and in the variable emissions used in the SAI models compared with the fixed reactivities employed in the emissions for the OZIPM models. The reactivities used in the OZIPM/CBM were determined from averages of emissions used in the trajectory model; for averaging the hydrocarbons aloft, a weighting factor was used each hour that was equal to the positive change in mixing height.

In a sense, the NO_2/NO_x ratio also acts as a reactivity effect. The OZIPM/CBM uses a fixed ratio of NO_2/NO_x (10 percent) for all NO_x emissions, whereas the SAI models allow this ratio to vary according to their source category (the average ratio is typically about 5 percent). At this time, we have not attempted either to change the OZIPM/CBM or to fix the ratio in the SAI model, because we feel the difference is trivial. For NO_x aloft, the OZIPM/CBM uses pure NO_2, which is close to typical values found in the trajectory model simulations because the NO_2/NO_x ratio is almost always greater than 0.85; often, the values are greater than 0.99.

> Integration Scheme. The OZIPM/CBM uses a Gear-type method without any steady-state approximations, whereas the trajectory model uses the same Crank-Nicholson finite

differencing scheme and steady-state approximations that are used in the Airshed Model. Again, this difference in model sophistication is opposite from the direction intended by our series of models. However, our previous tests using smog chamber experiments suggest that the differences introduced by the numerical integration schemes should be minimal.

> Vertical Layers. The Airshed Model and trajectory model share the same vertical layers and algorithms for numerical integration, but additional contributions are introduced into the Airshed Model for convergent or divergent winds. The OZIPM/CBM, of course, is limited to providing calculations of the mixed layer as a whole, but fixed concentrations in the layer aloft can be introduced as the mixing height rises. The SAI models account for mixing within the mixed layer, mixing within the inversion layer, and eddy diffusion among all layers. The OZIPM/CBM assumes instantaneous mixing within the entire mixed layer, and no eddy diffusion is considered across the boundary defined by the mixing height.

In our comparison studies, the effectiveness of multilayers and eddy diffusion was one of the central issues to be evaluated in this region of our model series. A problem that we tried to avoid, which does confound the comparison, is the entrainment of pollutants from aloft. The OZIPM/CBM requires fixed concentrations aloft, so these must be chosen from some "proper" average of the time-dependent concentrations computed in the SAI trajectory model. With the average value used in this study we attempted to weight most heavily the concentrations entrained when the mixing height rises most significantly. A more complex weighting scheme might involve the time when the greatest effect on the chemistry occurs; however, this effect was not evaluated. Concentrations aloft are not considered for the time before the inversion rises or after it has reached some maximum. As the mixing lid drops late in the afternoon, the only process affecting the surface layer from concentrations aloft is eddy diffusion. Eddy diffusion is treated in the Airshed Model and trajectory model, but is neglected in the OZIPM/CBM.

> Mixing height. All models used in the OZIPM/CBM that are based on the OZIPM computer code, as well as the Airshed Model and trajectory model, can use identical mixing

heights with values that vary linearly in time between specified values at each hour.

> Temperature. The temperature varies in the Airshed Model and trajectory model, but the OZIPM/CBM currently employs a fixed temperature. This difference can be significant. Temperature affects both vertical diffusion and chemistry in the SAI models, but it can affect only chemistry in the OZIPM/CBM because vertical mixing is assumed to occur instantaneously within the mixed layer.

> Emissions. The Airshed Model and trajectory model allow for emissions into all layers; the OZIPM/CBM treats all emissions in the mixing layer alike and does not directly address emissions above the mixing layer. For the layer aloft in the OZIPM/CBM, the emissions must be accounted for in the determination of the fixed concentrations aloft. The sum of the emissions used in the lower layers of the trajectory model was used for the mixing layer in the OZIPM-CBM. For this study, the OZIPM computer code was modified to treat emissions in an absolute fashion rather than as a multiple of the initial conditions. This was implemented by using the transported surface layer inputs as the initial concentrations. The normal initial concentrations (the CALC mode in OZIPM) were specified as 1.0 for both HC and NO_x, but these values were not added as initial concentrations. They were used only for emission fraction development because emissions are expressed relative to these values in the OZIPM code.

> Emissions for the SAI models are given as total moles emitted into each cell during each hour. To arrive at values appropriate for the OZIPM/CBM we used the following conversion procedure: the mixing volumes of the trajectory model and the OZIPM/CBM were assumed to be equal below the mixing height, such that

$$V = A \times Z_{mix} \quad ,$$

where A is the area of the horizontal cross-section of the air parcel defined in trajectory model simulations, and Z_{mix} is the mixing height. If the volume is expressed in cubic centimeters, the moles emitted in one hour (the number available from the trajectory model computer output) can be divided by this volume to give moles-cm^{-3}

units. This, in turn, can readily be converted to the OZIPM-CBM units of concentration, ppm, by using a conversion factor of 2.445×10^{10} ppm moles^{-1} cm^3, which is technically correct for a perfect gas at 298 K and 1 atmosphere of pressure. The numbers calculated at this point are almost directly applicable to the OZIPM/CBM model. First, the use of 1.0 for the initial concentrations of HC and NO_x in the CALC mode implies that each one-hour emissions number would be the concentration added during the hour if the mixing height were the same as the initial value Z_0. However, the computer codes are written so that, at each instant in time, the emissions factor is multiplied by Z_0/Z_{mix}. Therefore, the Z_{mix} drops out and the actual numbers (E_n) used are merely

$$En = A \times 2.445 \times 10^{10}/Z_0 \quad ,$$

where A and Z_0 are expressed in centimeters.

In this particular study, it was occasionally necessary to use special emissions factors. These factors were used for those cases in which the trajectory model employed substantial initial conditions for the first two layers (up to 100 m) even though the mixing height was only 50 m. Since there was typically an order-of-magnitude difference in concentration between the initial conditions below 100 m and the layers above this level, there was no way to compute a reasonable average value to be used in the OZIPM/CBM for the layer aloft. Therefore, the initial conditions between 50 and 100 m used in the SAI models were treated as emissions in the OZIPM/CBM. These "emissions" were added to the normal emission during the hour when the mixed layer in the SAI models jumped from 50 to 100 m. For these cases the appropriate OZIPM/CBM emissions factors merely add to the normal emissions, since the initial mixing height is 50 m and the height added is also 50 m.

3.2.1.3 Comparison of the OZIPM/CBM with the Standard City-Specific EKMA (OZIPP)

The obvious intention of this comparison was to evaluate only the differences between the Carbon-Bond chemistry used in the SAI models and the standard propylene/butane chemistry used in OZIPP. Although the OZIPM computer program was specifically written to handle such comparisons, some

complications were introduced when the OZIPP was operated with the propylene/butane chemistry. The Carbon-Bond chemistry used in this study assumes that formaldehyde and ketones represent half of the total aldehydes found in the simulation, whereas the formaldehyde in the city-specific EKMA is only 40 percent of the total amount of aldehydes. The photolysis rates used in the Airshed Model runs are based on a theoretical solar radiation function that does not contain the updated NO_2 absorption cross-sections. The city-specific EKMA simulations use the latest NO_2 cross-sections, which are approximately 13 percent lower than those used in the Airshed Model.

The reactivity of the two mechanisms was not typically adjusted in this study. The total HC concentrations and emissions rates were identical for these two models, but the standard EKMA propylene/butane chemistry was typically used with the standard 25 percent propylene, 75 percent butane, and 5 percent aldehyde reactivity.

Another difference between the OZIPM/CBM and the regular city-specific EKMA is the use of variable mixing-height inputs in the former, more sophisticated, version. In the OZIPM/CBM, instantaneous mixing heights are computed by linear interpolations between hourly input values rather than by the OZIPP method, which uses an exponential interpolation between the morning and afternoon mixing heights. The exponential increase in mixing height with time provides a constant dilution factor. In addition to the potential problems associated with the assumed shape of the mixing-height time profile, the standard OZIPP cannot consider a decrease in mixing height that may follow an increase, nor can it consider a resumption in mixing-height growth following a decrease or a pause.

In terms of modeling complexity, these models can be classified according to the levels of analysis described in the 1980 Federal Register notice on ozone modeling:

> SAI Airshed Model-Level I analysis using a complex grid model.

> SAI trajectory model-Level I analysis using a complex trajectory model.

> OZIPM/CBM-Level II analysis using a simplified trajectory model.

> City-Specific EKMA-Level III analysis.

3.2.2 Sacramento Case Studies

As previously described, the SAI Airshed Model was applied in Sacramento for two days--28 June and 24 August 1976. The SAI trajectory model was run for each day to establish the air parcel trajectory leading to each ozone maximum. Next, the results of the SAI trajectory model run were then used to develop the necessary input for the OZIPM/CBM (i.e., Level II) model. Finally, portions of the results from this model simulation were used to develop some inputs for the last model in the series--the city-specific EKMA. Each case study is described below.

3.2.2.1 Trajectory Calculations for 24 August 1976

The peak observed ozone level for 24 August 1976 was 0.13 ppm, and the SAI Airshed Model also predicted this level. The meteorology for that date consisted of relatively uncomplicated wind fields (i.e., low wind shear and little divergence). The SAI trajectory model was first run to determine the trajectory path to the maximum ozone predicted by the SAI Airshed Model; and the calculated trajectory is shown in figure 8. The detailed meteorological and emissions data used as input for the SAI trajectory model calculations are discussed in Reynolds et al. (1979). For this trajectory, the model predicted a peak ozone level (i.e., maximum one-hour average) of 0.13 ppm, which, as previously noted, agreed with both the observed level and with the prediction of the more complex SAI Airshed Model.

The SAI trajectory model simulation served as the basis for developing inputs for the OZIPM/CBM model simulation. From the SAI trajectory model output, we obtained the emission rates and meteorology (i.e., mixing heights) for each hour along the trajectory path. These data, used to derive inputs to the OZIPM/CBM, are summarized in table 3. The emission fractions, based on a column area of 4 km^2, were derived in accordance with the procedure described in the previous section. The initial conditions used in the OZIPM/CBM simulation are summarized in the top portion of table 4, along with the hydrocarbon reactivities. (Note that in this table, pollutants transported in the surface layer actually refer to initial concentrations, as was described in the previous section.) For this particular trajectory, the OZIPM/CBM predicted a peak ozone concentration of 0.14 ppm, slightly higher than that predicted by the two more complex models. Table 5 shows that the NO_x, PAR, ARO, and ozone concentration profiles for the SAI trajectory model and the OZIPM/CBM agree fairly well. This agreement implies that such factors as multilevel mixing, eddy diffusion, and elevated emissions are not particularly critical in this application.

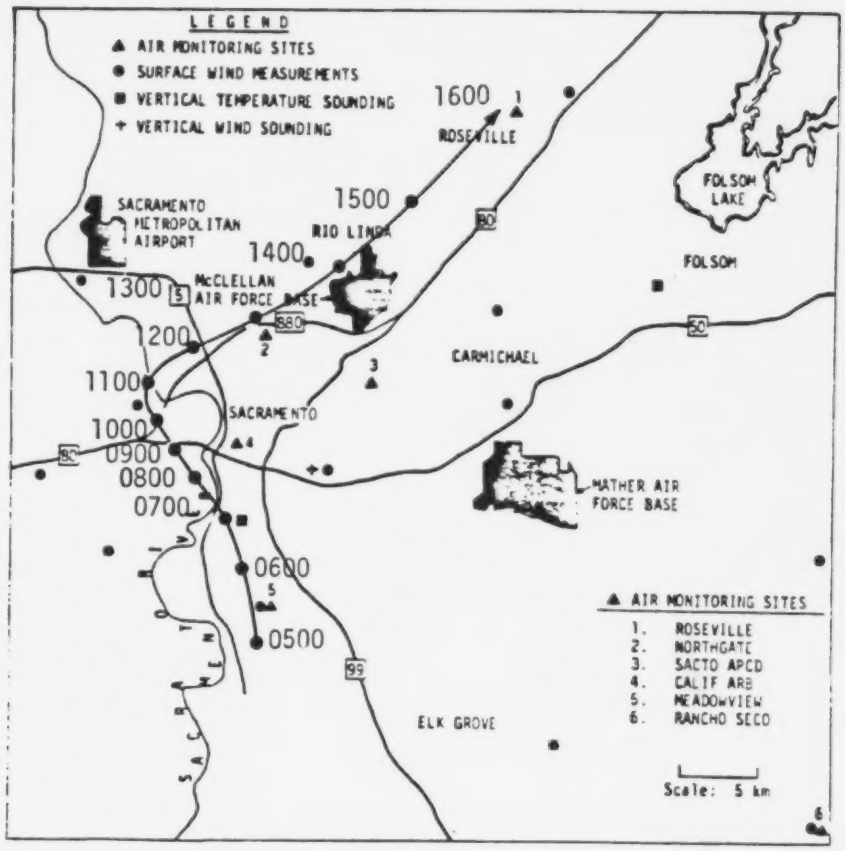

FIGURE 8. TRAJECTORY USED FOR 24 AUGUST 1976

TABLE 3. OZIPM/CBM EMISSIONS AND MIXING-HEIGHT INPUTS FOR 24 AUGUST 1976*

Time (PDT)	Emissions NO_x (ppm)	Emissions HC (ppmC)	Mixing Heights (meters)
0600	0.	0.	50
0700	0.00198	0.0031	50
0800	0.03287	0.2008	100
0900	0.144	0.904	150
1000	0.12225	0.556	225
1100	0.0194	0.157	300
1200	0.0074	0.123	650
1300	0.0287	0.0574	800
1400	0.0089	0.038	800
1500	0.01267	0.0463	800
1600	0.00709	0.0336	800
1700	0.01112	0.0766	800

* Taken from the SAI trajectory model calculation.

TABLE 4. INITIAL CONDITIONS FOR CALCULATIONS OF 24 AUGUST 1976*

(a) OZIPM/CBM

Transported Pollutants	NO_2/NO_x	NO_x (ppm)	HC (ppmC)	O_3 (ppm)
Surface†	0.518	0.0386	0.1594	0.0017
Aloft	1.000	0.00263	0.0552	0.0259

Hydrocarbon Reactivities:

	Emissions (percent of total)	Surface (percent of total)	Aloft (percent of total)
OLE	3.8	1.6	9.0
PAR	67.2	60.2	60.66
ARO	25.8	22.09	25.7
CARB	3.2	16.06	10.48

(b) City-Specific EKMA

	→ Species		
Transported Pollutants	NO_x (ppm)	HC (ppmC)	O_3 (ppm)
Surface†	0.0372	0.1881	0.0095
Aloft	0.0026	0.0552	0.026

NO_2/NO_x = 0.572.

Standard reactivity.

---

* Taken from the SAI trajectory model calculations.

† Transported pollutants in the surface layer refer to total initial conditions (i.e., local generation plus background plus any possible transported levels).

TABLE 5. COMPARISON OF THE SAI TRAJECTORY MODEL AND THE OZIPM/CBM CALCULATIONS FOR 24 AUGUST 1976 FOR NO_x, PAR, ARO, AND OZONE

Time (PDT)	NO_x		PAR		ARO		O_3	
	Trajectory	OZIPM/CBM	Trajectory	OZIPM/CBM	Trajectory	OZIPM/CBM	Trajectory	OZIPM/CBM
0600	0.039	0.039	0.096	0.096	0.018	0.018	0.002	0.002
0700	0.040	0.041	0.097	0.098	0.018	0.018	0.006	0.00004
0800	0.037	0.037	0.143	0.133	0.026	0.025	0.010	0.009
0900	0.068	0.071	0.285	0.299	0.055	0.056	0.011	0.013
1000	0.071	0.071	0.283	0.293	0.053	0.052	0.020	0.027
1100	0.053	0.052	0.234	0.242	0.041	0.040	0.041	0.053
1200	0.033	0.023	0.173	0.135	0.028	0.020	0.061	0.063
1300	0.024	0.017	0.139	0.114	0.020	0.015	0.078	0.078
1400	0.016	0.015	0.113	0.112	0.015	0.013	0.089	0.100
1500	0.015	0.013	0.113	0.112	0.013	0.011	0.108	0.117
1600	0.013	0.012	0.112	0.111	0.012	0.010	0.121	0.130
1700	0.013	0.011	0.114	0.112	0.011	0.009	0.129	0.139

The results of the OZIPM/CBM simulation were used to provide inputs for the city-specific OZIPP simulation. The lower portion of table 4 shows the initial conditions used in the simulation. City-specific OZIPP calculations require an initial and final mixing height. These values were 50 m and 800 m, and the inversion height lasted from 0800 to 1300 PDT. For OZIPP calculations we used standard reactivity (i.e., 25 percent propylene) for the hydrocarbon emissions splits and initial conditions. Figure 9 shows the results of the OZIPM/CBM calculation, including the station observations and the OZIPM/CBM predictions. The comparison between ozone observations and the OZIPM/CBM calculations shows that they are similar in temporal behavior. The ozone predicted by the city-specific OZIPP model was lower than the observed ozone concentration by about 7 percent.

3.2.2.2 Trajectory Calculations for 28 June 1976

OZIPM/CBM calculations for the 24 August 1976 trajectory just discussed were fairly straightforward because of the lack of wind shear. In contrast, the winds for 28 June 1976 contained high wind shears. The results and even the actual "paths" to ozone maximums can be quite different for the Airshed Model and trajectory model if wind shear or any horizontal dispersion occurs in the Airshed Model. The trajectory calculations for 28 June attempt to address the problems of wind shear and horizontal dispersion because these factors can be important in comparisons of trajectory and grid modeling results.

We used the trajectory model to generate a back-trajectory from the point of maximum ozone. Even though this trajectory model employs the same number and size of the vertical layers as the Airshed Model, the computer algorithm that is used to run the back-trajectories follows only the surface winds of the grid model. The wind shear within the mixing layer was significant for this day, and ignoring the winds in the second layer generated a back-trajectory that would have been inappropriate since the surface winds did not pass over any major emissions. Because good mixing typically occurs within the mixed layer, we modified the computer algorithm of the trajectory model to average the winds within the mixed layer and used the average value instead of the surface wind value only. This produced the trajectory shown in figure 10, which led to an ozone prediction of 0.15 ppm at 1700 PDT.

The maximum observed ozone of 0.16 ppm occurred near Northgate at 1500 PDT; the Airshed Model predicted a maximum of 0.15 ppm at 1600 PDT between Northgate and Roseville. Since the trajectory model predicted an ozone peak of 0.15 ppm at 1700 PDT, an hour later than the prediction of the Airshed Model, we could not readily compare the EKMA models (OZIPM/CBM

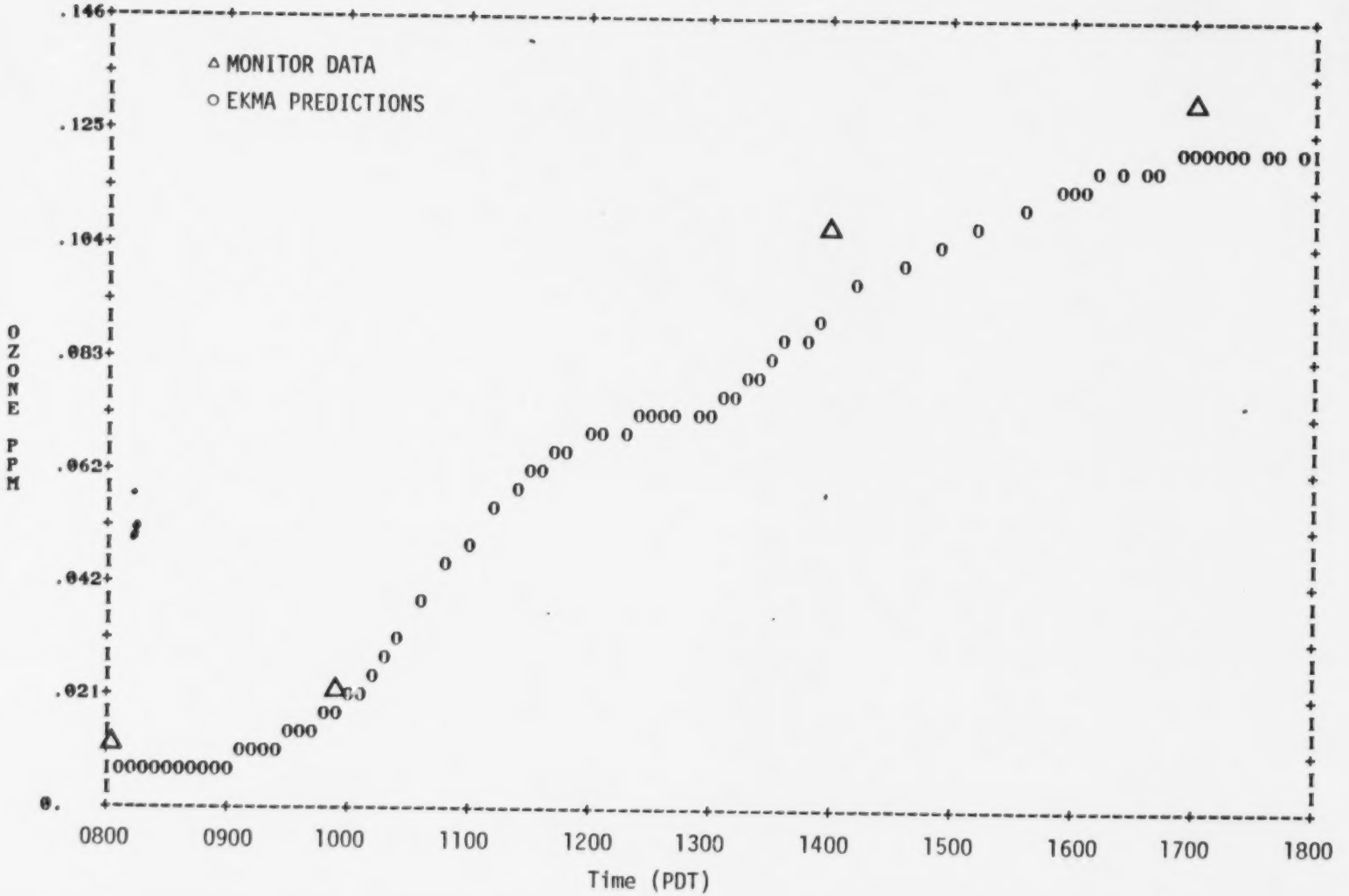

FIGURE 9. COMPARISON OF OZONE BETWEEN STATION OBSERVATIONS AND MODEL PREDICTIONS FOR CITY-SPECIFIC EKMA FOR 24 AUGUST 1976--SACRAMENTO

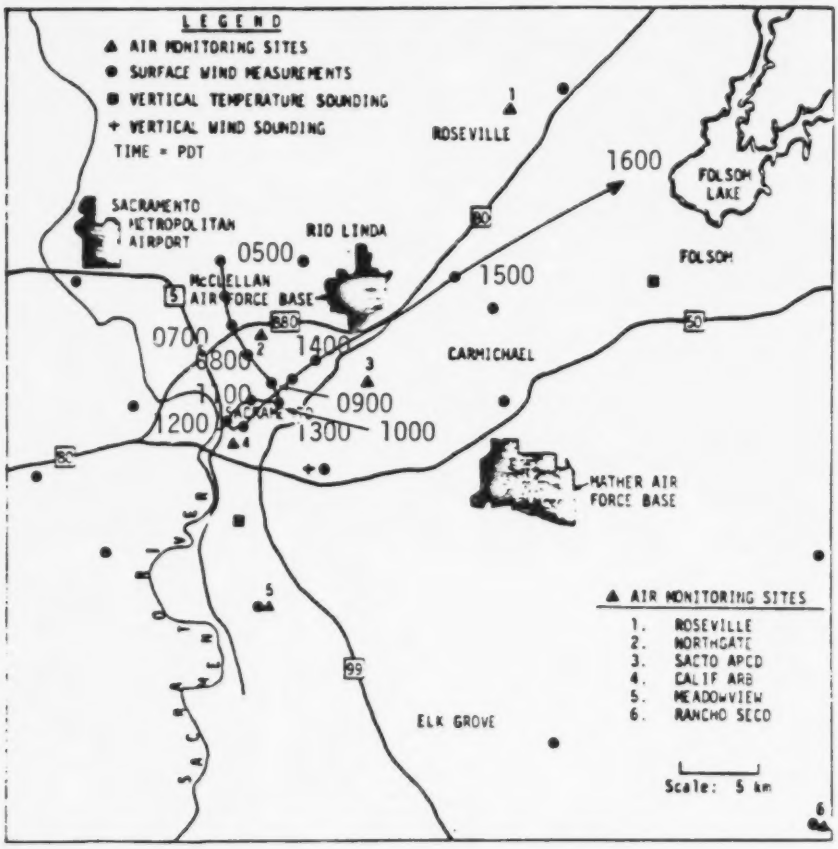

FIGURE 10. TRAJECTORY USED FOR 28 JUNE 1976

or city-specific) with the airshed predictions. Instead, we compared the predictions of the OZIPP-type models to the trajectory model predictions only.

From the trajectory model results, we obtained the emissions rates and mixing height information needed to perform the OZIPM/CBM calculations as discussed for the 24 August 1976 calculations. Table 6 shows the emissions rates and mixing heights used in the OZIPM/CBM calculations. The top portion of table 7 shows the initial conditions used in the OZIPM/CBM calculations. The OZIPM/CBM simulation resulted in a peak ozone concentration of 0.16 ppm, which, like the 24 August simulation, was slightly higher than the SAI trajectory model predicted.

As for the cases previously discussed, the inputs for the city-specific EKMA were derived from the OZIPM/CBM simulation. To provide a direct comparison between the models, 0800 PDT OZIPM/CBM conditions were taken as the initial conditions for the city-specific OZIPP simulation.

Figure 11 shows the results of the city-specific OZIPP calculation for ozone. The observed ozone at the monitoring stations along (or near) the trajectory is also shown in this figure. Unfortunately, the trajectory passed over only a few stations, and these do not record the ozone maximum; therefore, we were unable to compare the observed ozone maximum with the model-predicted ozone maximum. The city-specific OZIPP simulation was carried out for 10 hours, from 0800 PDT to 1800 PDT, whereas the trajectory model ran from 0600 PDT to 1700 PDT. The trajectory model predicted an ozone level of 0.15 ppm at 1700 PDT. The OZIPM/CBM, a model that is more general (i.e., it employs a variable mechanism, variable mixing heights, etc.), predicted an ozone level of 0.167 ppm at 1700 PDT. The city-specific EKMA (standard OZIPP) predicted an ozone of 0.13 at 1800 PDT.

3.2.3 Summary of Results for Sacramento Case Studies

Table 8 summarizes the results of the case studies just described. The important conclusion reached in this part of the study is that the simple OZIPP-type trajectory model can produce simulations that agree very closely with the simulations of highly sophisticated models such as the SAI Airshed Model and the SAI trajectory model. Indeed, the present study involved the use of extremely detailed input data common to all models; yet, the main differences in results were due to the differences in chemistry between the OZIPM/CBM and the OZIPP model with the regular propylene/butane chemical mechanism.

TABLE 6. EMISSION RATES AND MIXING HEIGHTS USED IN THE OZIPM/CBM CALCULATIONS FOR 28 JUNE 1976*

Time (PDT)	Emissions NO_x (ppm/hr)	Emissions HC (ppmC/hr)	Mixing Heights (meters)
0600	0.	0.	150
0700	0.00067	0.0011	150
0800	0.00217	0.008	220
0900	0.01171	0.0388	250
1000	0.01466	0.07805	280
1100	0.02545	0.1173	310
1200	0.02618	0.10678	370
1300	0.0333	0.09757	460
1400	0.04198	0.20355	600
1500	0.03253	0.13898	800
1600	0.03584	0.10951	800
1700	0.02019	0.04486	800

* Taken from SAI trajectory model calculations.

TABLE 7. INITIAL CONDITIONS USED IN THE CITY-SPECIFIC EKMA CALCULATIONS OF 28 JUNE 1976*

(a) OZIPM/CBM

Transported Pollutants	NO_2/NO_x	NO_x (ppm)	HC (ppmC)	O_3 (ppm)
Surface	0.845	0.0457	0.2899	0.0019
Aloft	1.000	0.0025	0.0541	0.649

Hydrocarbon Reactivities:

	Emissions (percent of total)	Surface (percent of total)	Aloft (percent of total)
OLE	4.0	2.6	0.9
PAR	67.5	48.6	63.8
ARO	26.0	13.0	25.8
CARB	2.5	35.7	9.6

(b) City-Specific EKMA

	Species		
Transported Pollutants	NO_x (ppm)	HC (ppmC)	O_3 (ppm)
Surface	0.0319	0.218	0.035
Aloft	0.002	0.054	0.065

NO_2/NO_x = 0.773

Standard reactivity.

* Taken from the SAI trajectory model calculations.

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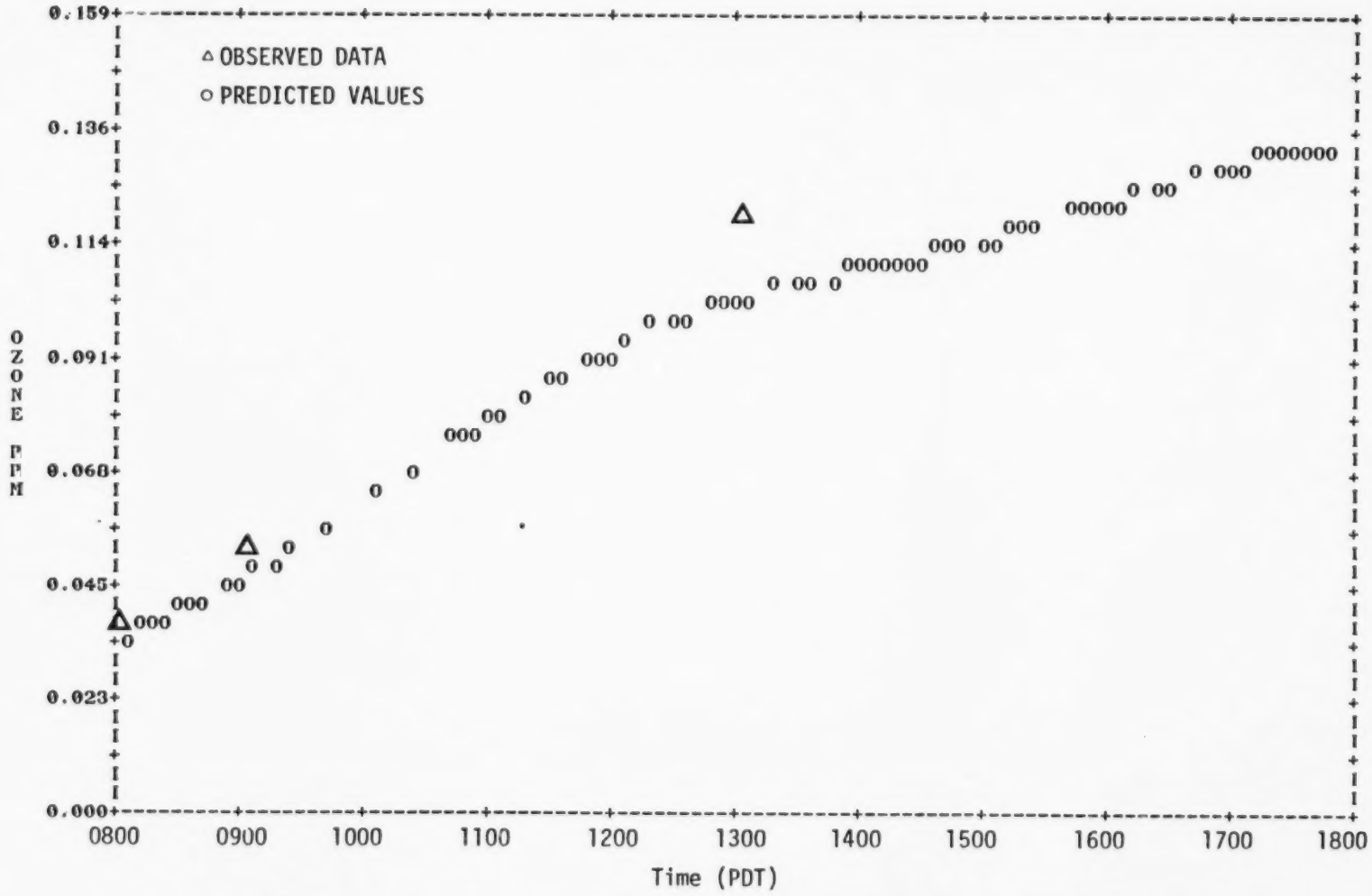


FIGURE 11. COMPARISON OF OZONE BETWEEN STATION OBSERVATIONS AND MODEL PREDICTIONS FOR 28 JUNE 1976--SACRAMENTO

TABLE 8. COMPARISON OF OZONE PREDICTIONS FOR FOUR DIFFERENT MODELS ON 28 JUNE 1976 AND 24 AUGUST 1976 IN SACRAMENTO

Date (1976)	Observed Maximum Ozone (ppm)	Time to Observed Maximum O_3 (PDT)	Airshed Model Maximum O_3 (ppm)	Time to Peak (PDT)	Trajectory Model Maximum O_3 (ppm)	Time to Peak (PDT)	OZIPM/CBM Maximum O_3 (ppm)	Time to Peak (PDT)	City-Specific EKMA Maximum O_3 (ppm)	Time to Peak (PDT)
28 June	0.16	1500	0.15	1600	0.15	1700	0.16	1700	0.13	1700
24 August	0.13	1700	0.13	1700	0.129	1700	0.139	1800	0.121	1800

Whereas the complicated emissions data constituted the unique feature of the San Francisco study, the highlight of the Sacramento study is the complex wind shear of the 28 June 1976 simulations. The simple averaging of wind data for the two cells within the mixing layer simulated in the SAI grid model seemed to generate reasonable ozone levels in the trajectory models. Therefore, the studies of the simple trajectory models conducted to date appear to show that if the precursor levels of HC and NO_x were similar in either the complex or simple models, the chemical mechanism, especially if it's the same mechanism, tends to simulate similar levels of ozone. Although this conclusion seems obvious, obtaining similar precursor levels for the complex and simple models is by no means straightforward.

The present study involved the use of detailed computer outputs from the SAI Airshed Model and the trajectory model. These outputs served as sources of input, standards of performance, and guides to the treatment of inputs. Of course, typical applications of the EKMA would not be made in such an environment. However, the indications of this study are that careful application of a simple model such as the OZIPP-type trajectory model can lead to reasonable ozone simulations. If the local situation indicates complex problems such as diverse emissions densities or wind shear, extra care is warranted. In the following section we explore the sensitivity to some of the situations previously discussed; in section 5 we use isopleths to examine the relative applications of EKMA.

4 SENSITIVITY STUDIES

In this evaluation, the emphasis on sensitivity is related to performance in an absolute sense rather than in the relative sense that is used in the control-strategy application of the EKMA. Therefore, we are concerned with the absolute ozone values simulated by the simple OZIPP trajectory model. In the San Francisco region sensitivity to OZIPP parameters and inputs was emphasized, whereas in the Sacramento study (discussed later in this chapter) sensitivity to differences between models was emphasized.

We did not use a systematic approach to selecting the input parameters of OZIPM; instead, we emphasized the regional aspects of the cities studied. For example, the EKMA procedure for predicting control requirements necessitates a knowledge of the initial (0600 to 0900) HC/NO_x ratio. Yet, the application of the model to the San Francisco region indicates that the initial HC/NO_x ratio, or more important, the initial concentrations of HC and NO_x, do not affect the simulated maximum ozone values. Hence, the use of observed HC/NO_x ratios may be questionable for the isopleth application of the EKMA to San Francisco, even though the trajectory model used in the approach can provide reasonable simulations of episode ozone levels in the area. The conclusion that observed HC/NO_x data for San Francisco are questionable hinges on the accuracy of the trajectories determined for this study, the central issue being the origin of all trajectories in the Pacific Ocean at 0800. When some trajectories starting in the city at 0800 were investigated, the combination of observed wind velocities and low HC/NO_x ratios in both the observations and the emissions inventory produced ozone peaks late in the day far downwind of the region. These trajectories had passed the monitoring sites before the occurrence of the observed maximum ozone concentrations. Since there were no monitoring sites with which to test the model, the trajectories were not studied further. Trajectories that originate in the urban core and arrive at the monitoring site at the proper time do not necessarily coincide with trajectories derived from surface wind measurements. However, it must be emphasized that significant uncertainties are associated with the latter, especially in areas of complex wind flow.

4.1 THE SAN FRANCISCO REGION

4.1.1 Initial Conditions

The main inputs to the OZIPP or the OZIPM that control the ozone development for the San Francisco trajectories are the emissions and mixing-height profiles. According to our analysis, all trajectories that lead to high ozone formation originate over the Pacific Ocean. To illustrate the lack of sensitivity to initial conditions, the trajectory to Livermore was simulated using a wide range of initial concentrations and ratios for HC and NO_x from 26 July 1973. The results are shown in table 9. The emissions profiles were recomputed for each calculation so that the absolute level of precursor concentrations caused by emissions was identical for all the cases. Similar insensitivity to initial conditions would be seen in the other San Francisco trajectories since they all originate over the ocean. This is not a case for generally ignoring initial conditions in OZIPP models, because other cities do not often experience the wind velocities and clean upwind air found in San Francisco. The point we wish to emphasize here is that the OZIPP-type model can still give reasonable results in spite of this lack of sensitivity to initial conditions.

4.1.2 Mixing Heights

The mixing-height profiles, typically available directly from the LIRAQ files, were investigated for sensitivity in two ways. First, the necessity of using the OZIPM option of hourly mixing-height data was explored relative to using the normal city-specific EKMA version in OZIPP, in which only initial and final mixing heights are used. This area of sensitivity proved to be irrelevant for this study, because the change in mixing height with time could, in general, be closely simulated by the proper choice of initial and final mixing heights for the standard OZIPP input parameters. In other studies, such as those of Whitten and Hogo (1981), trajectories have been considered in which the shape of the mixing height with time could not be adequately simulated using the standard OZIPP parameters. The second method involved the concept of mixing height itself (discussed in detail in the previous chapter). The LIRAQ simulation of 26 July 1973 was used extensively by the BAAQMD for the AQMP. The main trajectory studied here, on the basis of the meteorological data found in the LIRAQ files, arrived at the site of maximum observed ozone--Livermore--on that date. Because of the significance of this trajectory, special treatment of the OZIPM input data for mixing heights seemed appropriate. However, determination of the "proper" mixing height data was not pursued beyond the following sensitivity study. Several mixing

TABLE 9. VALUES FOR MAXIMUM OZONE VERSUS VALUES FOR INITIAL CONDITIONS*

NO_x (ppm)	HC (ppmC)	Maximum Ozone
0.003	0.03	0.197
0.003	0.01	0.196
0.003	0.003	0.194
0.001	0.03	0.198
0.001	0.01	0.196
0.001	0.003	0.195
0.0003	0.03	0.197
0.0003	0.01	0.195
0.0003	0.003	0.195

* 26 July 1973 trajectory No. 1.

heights were adjusted for the later stages of the day when the air parcel passed through a canyon area into the Livermore valley where the ozone maximum was observed. Results using the different mixing-height profiles or vectors are shown in figure 12.

4.1.3 Emissions Vector (Wind Speed)

Sensitivity to mixing-height input data is rather straightforward in the OZIPM model. Precursor concentrations are reduced linearly as the mixing heights are increased relative to the initial mixing height. Ozone is reduced, but less than linearly, with dilution (Fox, Kamens, and Jeffries, 1975). In some cases, a large concentration of ozone aloft can actually lead to increases in ozone as the mixing height rises.

Sensitivity to the emissions-profile data actually involves input preparation factors such as wind speed and model size. The wind-speed factor was of paramount importance for the San Francisco trajectories because this area is characterized by sharply contrasting emissions densities. The dominant westerly winds typically bring clean air into the area from the Pacific Ocean. The city itself lies on the northern end of a peninsula and is thus surrounded by water on three sides. The peninsula is a heavily populated suburban area. Across San Francisco Bay, to the east of the city, are the large urban and suburban areas of Oakland. Just to the east of this populated area are hills. Hence, a typical air parcel in this area is subjected to sharply contrasting emissions levels. If a low wind speed is associated with the air parcel, the time spent over areas of high emissions is much longer.

For areas such as Los Angeles, there is much less contrast in emissions levels along a trajectory path once the air parcel reaches land. Wind speed would be less critical for an air parcel passing over a large area of uniform emissions density. Hence, wind speed in the San Francisco region is much more important than it is in the Los Angeles region.

This sensitivity to wind speed is demonstrated in the 26 July 1973 trajectory to Livermore by using twice the reported speed during the morning hours. Figure 13 shows that a significant change is noted in the ozone profiles for different assumed wind speeds.

4.1.4 Model Size

The grid squares of the LIRAQ model were of 5-km size, the value that we used to define the narrowest width of the OZIPM trajectory model. Since the path determined by our analysis of the LIRAQ wind data did not

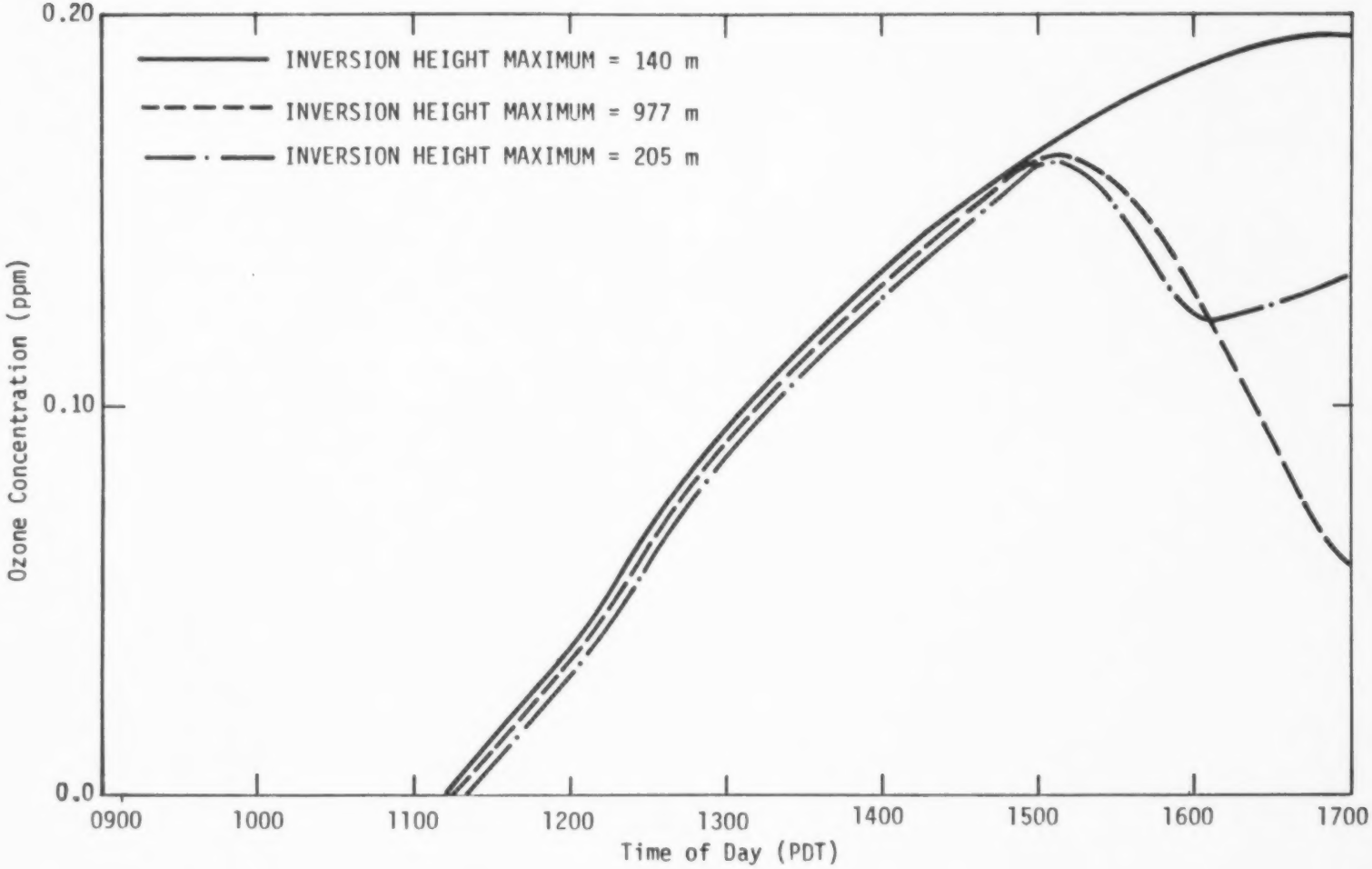


FIGURE 12. EFFECTS OF INVERSION HEIGHTS ON MAXIMUM OZONE PRODUCED: 26 JUNE 1973, TRAJECTORY 1.

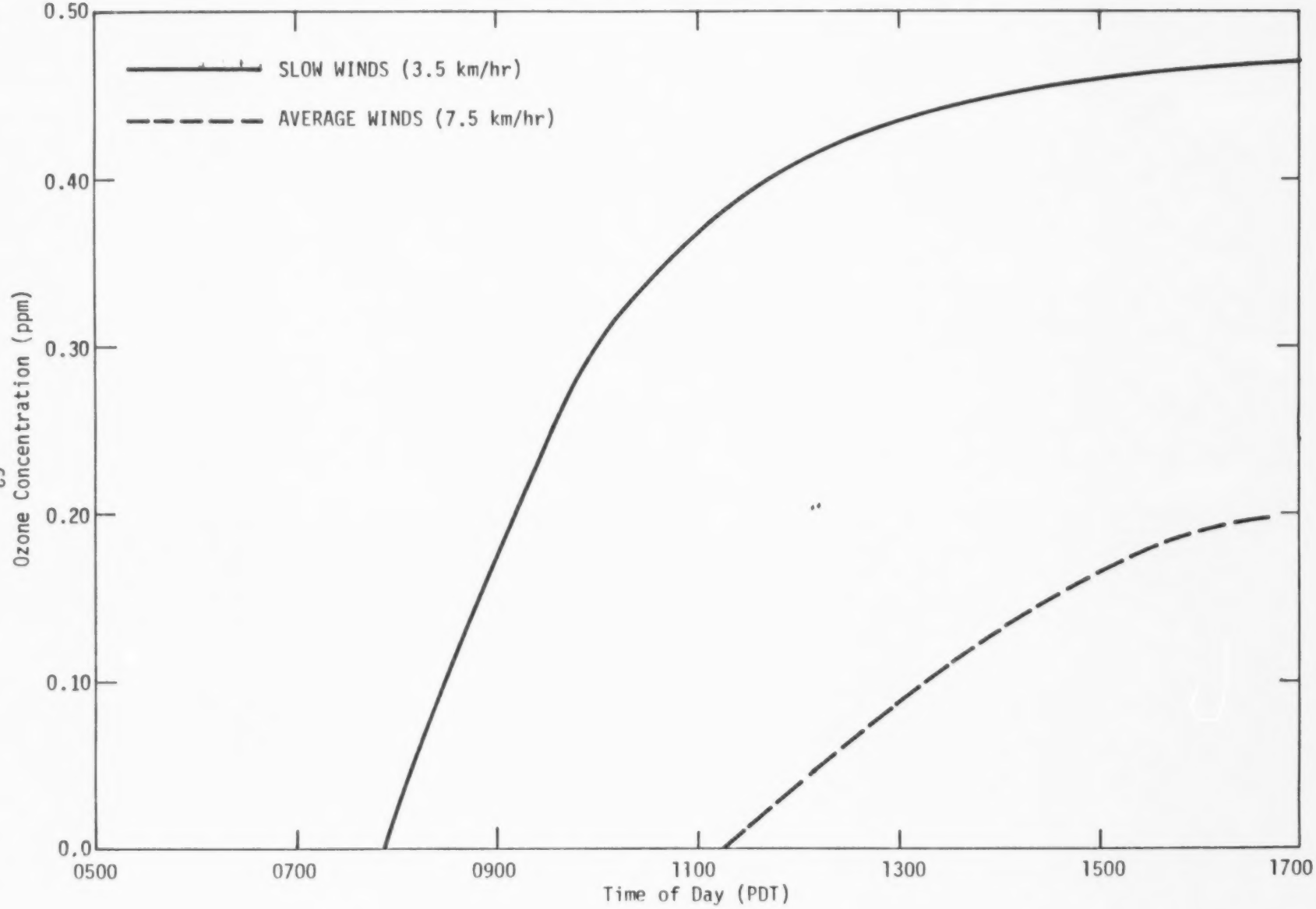


FIGURE 13. EFFECTS OF WIND SPEED ACROSS SAN FRANCISCO ON OZONE PRODUCTION: 26 JUNE 1973.

generally follow the regular grid pattern of the LIRAQ model, we determined the emission information for the OZIPM inputs by including adjacent grid-square information when the trajectory path width overlapped the LIRAQ grid squares. The adjacent information was averaged using simple linear weighting.

Although the adjacent grid trajectories produce large differences in ozone concentrations, the 15-km trajectory produces results similar to those for the central 5-km trajectory, as shown in figure 14. The size of San Francisco--roughly 15 km--tends to place an upper limit on the nominal size of a reasonable model. Also for this sensitivity analysis, the paths of the trajectories were "forced" to follow the central, or standard, path. Actually, an analysis of the wind patterns indicates that the path to the north of the standard path turned toward the north and crossed San Francisco Bay; thus, the high urban emissions did not affect the Livermore valley. Therefore, this sensitivity analysis involves more than a simple change in width: the high value of 0.48 ppm ozone predicted for the adjacent trajectory to the north reflects a sensitivity to path definition as well.

4.2 THE SACRAMENTO REGION

The SAI Airshed Model and trajectory model had previously been applied to this area and, therefore, detailed inputs and outputs were readily available and familiar to us. This access enabled us to conduct a comparison study emphasizing individual differences between the SAI models and OZIPP-type models. A similar study was recently completed for the Los Angeles area by Whitten and Hogo (1981). The present evaluation involved a series of four models that varied in complexity from the SAI Airshed Model to the regular city-specific EKMA trajectory model found in the OZIPP computer code. Two were OZIPP-type models, one was the regular OZIPP model, and the fourth was based on the OZIPM version and was further divided as follows:

> The city-specific model employing variable, instead of constant, dilution rates. The OZIPM computer code was needed for this exercise.

> The OZIPM model using variable dilution rates and the same Carbon-Bond chemistry used in the Sacramento airshed modeling study (i.e., OZIPM/CBM).

> An OZIPP-type model that we have called OZIPM/CBM. Along with the variable dilution and CBM chemistry additions, the starting time is changed to be early enough in the

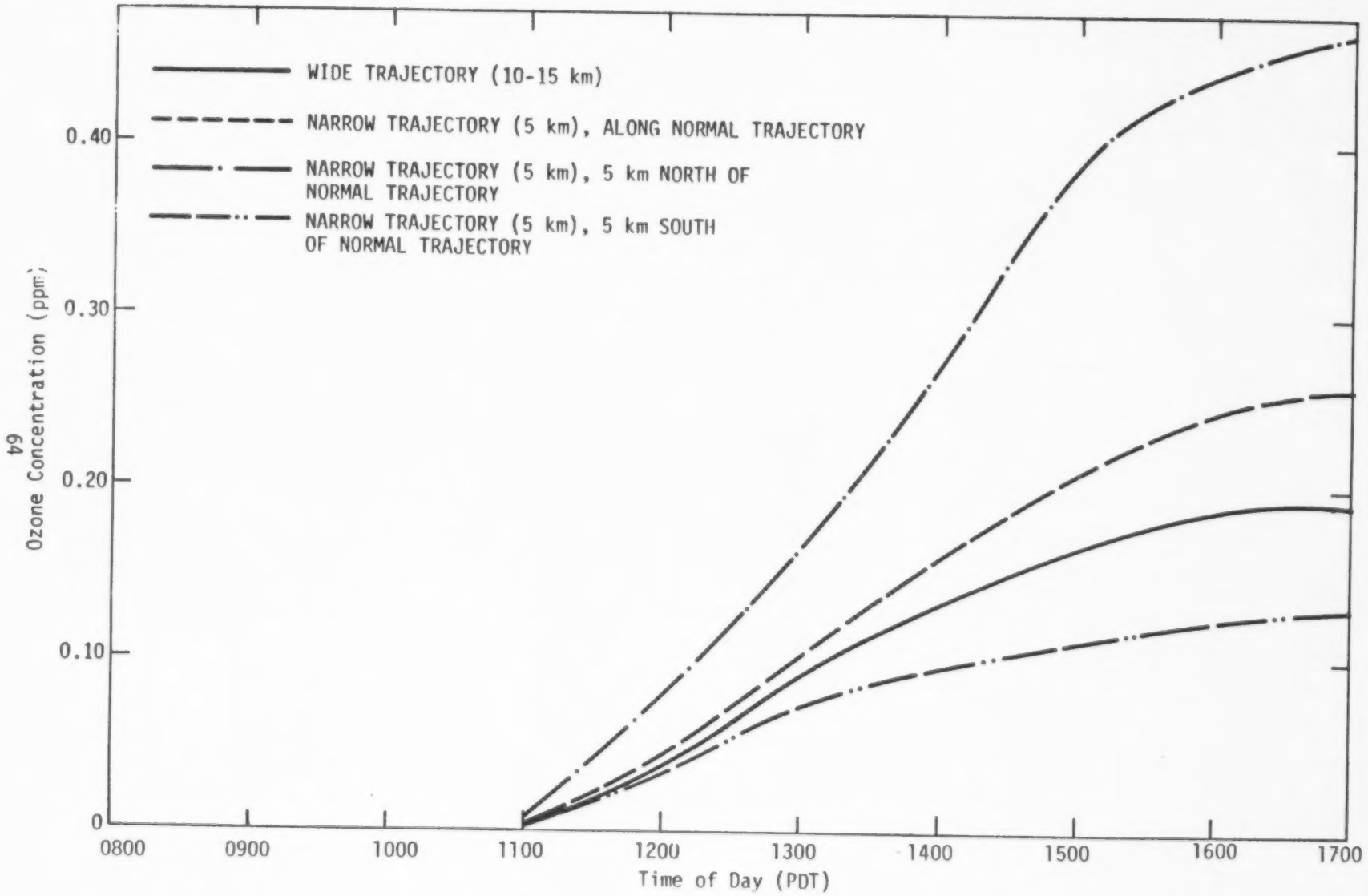


FIGURE 14. EFFECTS OF TRAJECTORY WIDTH ON MAXIMUM OZONE: 26 JULY 1973

morning to maximize the influence of the emissions inventory. In the regular, city-specific OZIPP, the 0800 starting time is intended to maximize the influence of the 0600 to 0900 precursor concentrations.

The model series was intended to demonstrate the sensitivity of OZIPP-type models to three factors: dilution, chemistry, and starting time. Although different starting times were used in practice, the comparisons of this study remove such a difference. The model employing a starting time of 0800 PDT used initial conditions that were generated at 0800 by the model that was started earlier. The model that had been started earlier could, therefore, conceivably be restarted at 0800 to produce the same result produced by the continuous model version. The differences between models due to the dilution factor (variable versus constant) were also unimportant in this study because the shapes of the variable dilution curves could, in general, be closely approximated by using a constant dilution rate. For instance, a calculation was made for 24 August 1976 in Sacramento using the city-specific inputs with both variable dilution and constant dilution rates, but no difference in ozone predictions occurred between the two simulations.

As indicated in chapter 3 of this report, though starting time and variable dilution factors did not show any important sensitivity for the Sacramento case, the change in chemical mechanism did have a noticeable effect. More ozone was generated by the CBM chemistry than by the standard EKMA chemistry, an effect that is consistent with the results reported by Whitten and Hogo (1981). That study further demonstrated that the standard EKMA chemistry could be easily modified to significantly increase the calculated peak ozone. The only real option available in the standard OZIPP model with which to enhance ozone is reactivity, since the other options are limited by observations. The computer code was also slightly modified to accept higher photolysis rates for aldehydes. Both of the adjustments (reactivity and higher photolysis rates) merely accelerated the production rate of simulated ozone during the morning hours (which was already higher for the standard EKMA chemistry than for the CBM chemistry), but the final ozone peak was not significantly enhanced. No attempts to modify the CBM chemistry were made because all models (the grid, trajectory, and OZIPM/CBM models) using it produced results whose differences (when they occurred) could be explained by factors other than chemistry.

An important aspect of the differences in chemistry is found in the control requirements predicted by the two chemical mechanisms. This aspect is discussed in the next section, which details EKMA applications. Absolute differences in simulated peak ozone between the mechanisms are often less important when they are used with the relative method of EKMA.

5 EKMA APPLICATIONS

When the EKMA is applied to an urban area, isopleth diagrams, observed HC/NO_x ratios, and observed ozone maximums are used to estimate the emissions control requirements that are necessary to achieve compliance with the ozone standard. The isopleth diagrams for use in EKMA applications are constructed by interpolating between multiple simulations of a specific trajectory model. Normally, the ordinate and abscissa of the isopleth diagrams represent the initial conditions of HC and NO_x concentrations used in the trajectory model simulations. The EKMA isopleth lines represent constant maximum one-hour ozone simulated by the trajectory model from the ordinate and abscissa value for initial conditions. These diagrams are constructed by the OZIPP and OZIPM computer programs.

In previous sections of this report, we discussed versions of the OZIPP trajectory model as it was applied in the absolute sense. That is, we were concerned with the absolute value of ozone predicted by the model from given initial precursors, emissions, and meteorological factors. When the trajectory model is used via the isopleth diagram, the model is used in a relative fashion. The starting point on the diagram is the intersection of the ozone isopleth line corresponding to the observed ozone maximum with the radial line corresponding to the observed HC/NO_x ratio for 0600 to 0900 hours. The ordinate and abscissa values are intended to relate to percentage changes in the HC and NO_x emissions inventories.

In this section we discuss the uncertainties associated with the construction and use of the EKMA isopleth diagrams. Whereas we previously compared (in an absolute sense) individual trajectory model simulations with those of various other models and with observations, in this section we compare (in a relative sense) the changes in ozone predicted by various models on the basis of percentage changes in emissions.

5.1 CONSIDERATIONS RELATED TO THE USE OF ISOPLETH DIAGRAMS

5.1.1 Fixed Monitoring Sites

The time and location of maximum observed ozone concentrations can change as a result of a change in emissions only. Grid models typically show such effects. The probability of the coincidence of monitoring sites and the actual location of maximum ozone concentrations can either increase or decrease as a result of changes in emissions. The proper deployment of several monitoring sites and the application of numerous trajectory paths can, to some extent, mitigate this problem. The use of a grid model is also helpful.

Another related problem occurs when winds vary in direction during the course of a day because the air arriving at a monitoring site can originate at several different locations. If the proposed control strategy alters the time of occurrence of the ozone maximum, the base trajectory utilized to construct the isopleth diagram then becomes inappropriate for the monitoring site. When the wind directions are constant throughout the day, a change in ozone peak timing merely lengthens or shortens the path to the monitoring site.

5.1.2 Uneven Changes in Emissions

Mobile-source emissions are, for the most part, regulated at the federal level, whereas stationary sources are more often subject to local control. Therefore, because the federal controls may be different from the local requirements and because some areas are dominated by mobile sources and others stationary sources, the uniform control of either HC or NO_x is rarely even in time and space. Individual trajectory-model simulations might provide acceptable levels of accuracy for the base-case year and the future year because these models can typically alter the timewise distribution of emissions input data. However, the isopleth approach requires some uniform emission pattern for all points on the diagram.

Depending on the level of sophistication, some trajectory models can also account for changes in hydrocarbon reactivity along the trajectory path. However, in constructing isopleth diagrams, considering changes in both emissions patterns and reactivity is beyond the scope of the present algorithms.

5.1.3 Transported Pollutants

The regular city-specific EKMA isopleth algorithm uses the same amounts of transported pollutants for all points of the diagram. In practice, the regulation of mobile emissions at the federal level would modify the transportation of pollutants. It was shown by Whitten and Hogo (1981) that on the basis of the EKMA, significant differences in control requirements can result from different assumptions about the transported pollutants in the surface layer and the layer aloft. The latest guidelines for using the EKMA suggest employing two isopleth diagrams to deal with this problem.

5.2 SAN FRANCISCO APPLICATIONS

The AQMP (1979), using the LIRAQ model, offers a unique means of evaluating the EKMA. The control-strategy LIRAQ predictions for various scenarios can be directly contrasted with comparable EKMA predictions. We have also included brief discussions of two other topics involving the use of EKMA in the San Francisco region:

> Isopleths prepared from some of the widely differing initial conditions discussed in section 4, which demonstrated a lack of sensitivity to initial conditions (see table 9).

> A comparison of isopleths using the CBM and the standard EKMA chemical mechanisms.

> A comparison of isopleths generated assuming different trajectories.

5.2.1 Basic Comparisons between LIRAQ and EKMA

Several control scenarios were described in the AQMP (1979). For cases in which comparisons could be made with the EKMA, we constructed isopleth diagrams and applied various estimates of predicted ozone concentrations using the EKMA technique. In this section, attention is focused on those EKMA applications:

> The OZIPM trajectory analysis described in chapter 3 (i.e., a Level II analysis).

> A basic city-specific EKMA analysis using current guidelines for a Level III analysis (EPA, 1980).

> A basic city-specific EKMA analysis in which the Carbon-Bond Mechanism was substituted for the standard propylene/butane chemistry contained in OZIPP.

Table 10 shows the comparative results for the different scenarios applied in the LIRAQ analysis. A discussion of these results follows.

For the LIRAQ evaluations, 26 June 1973 was selected as the prototype meteorological day. The trajectory corresponding to the prototype day was shown earlier in figure 1. The OZIPM computer code was used to construct the isopleth shown in figure 15 since the starting times and hourly mixing height inputs were not the standard ones assumed for the city-specific EKMA. The results indicate that the Level II predictions are generally less sensitive to changes in hydrocarbons and/or NO_x than are the LIRAQ predictions. Because of the fundamental differences in the two models, explanations for these differences cannot be postulated. However, the sensitivity of Level II predictions is addressed in the next section.

The isopleth approach is, in effect, confined to one trajectory path, whereas the grid models cover essentially all possible trajectories in space and time. Thus, the worst case found over the entire gridded area would normally be found in the grid model rather than (for this case) in three trajectory paths. This reasoning leads to some surprising comparisons of LIRAQ (grid) and EKMA (trajectory) results. For 20, 40, and 60 percent HC reduction scenarios, plus the scenarios combined using reductions of 40 percent HC and 20 percent NO_x, the ozone predictions from LIRAQ are lower than those from the EKMA. The remaining three scenarios (80 percent HC reduction, and 40 percent NO_x reduction) reflect a situation in which the worst case over the gridded area is higher than, or equal to, the worst case along the specific trajectory.

Two additional isopleth diagrams for 26 July 1973 were constructed to reflect the current guidelines for a city-specific EKMA analysis (i.e., a Level III analysis). In this approach, a trajectory is followed from the urban core to the site of the observed peak ozone level (EPA, 1980). The isopleth diagram shown in figure 16(a) was constructed using the city-specific EKMA program (i.e., OZIPP), which reflects the standard propylene/butane chemistry contained in city-specific EKMA. Figure 16(b) was constructed using the Carbon-Bond Mechanism rather than the standard chemistry. The inputs for both diagrams, which are summarized in table 11, correspond to conditions for 26 July 1973.

The HC/NO_x ratio for the Level III applications was derived from 0600-to-0900-hour-averaged HC and NO_x observations taken at the downtown San Francisco monitoring station (MacCracken and Sauter, 1975). The monitoring station reported total hydrocarbons only, but methane

TABLE 10. CONTROL-STRATEGY COMPARISONS FOR SAN FRANCISCO BETWEEN LIRAQ AND EKMA APPLICATIONS*

Models Studied	Reduction (percent) HC / NO_x	0 / 0	20 / 0	40 / 0	60 / 0	80 / 0	40 / 20	80 / 40	0 / 40
LIRAQ predictions		0.189	0.140 (-26%)	0.082 (-57%)	0.069 (-63%)	0.055 (-71%)	0.119 (-37%)	0.064 (-66%)	0.233 (+23%)
OZIPM (Level II) (based on 0.189 max.)		0.189	0.161 (-15%)	0.145 (-23%)	0.102 (-46%)	0.036 (-81%)	0.141 (-25%)	0.062 (-67%)	0.160 (-15%)
Level III EKMA (based on 0.189 max.)		0.189	0.130 (-31%)	0.080 (-57%)	<0.080 (<-57%)	<0.080 (<-57%)	0.10 (-47%)	0.08 (-57%)	0.247 (+31%)
Level III EKMA using CBM (based on 0.189 max.)		0.189	0.112 (-41%)	<0.08 (<-57%)	<0.08 (<-57%)	<0.08 (<-57%)	0.08 (-57%)	<0.08 (<-57%)	0.313 (+66%)

* The predicted ozone level is shown for each control scenario in addition to the percentage change from the base-case level (i.e., no HC or NO_x reductions).

32R/14

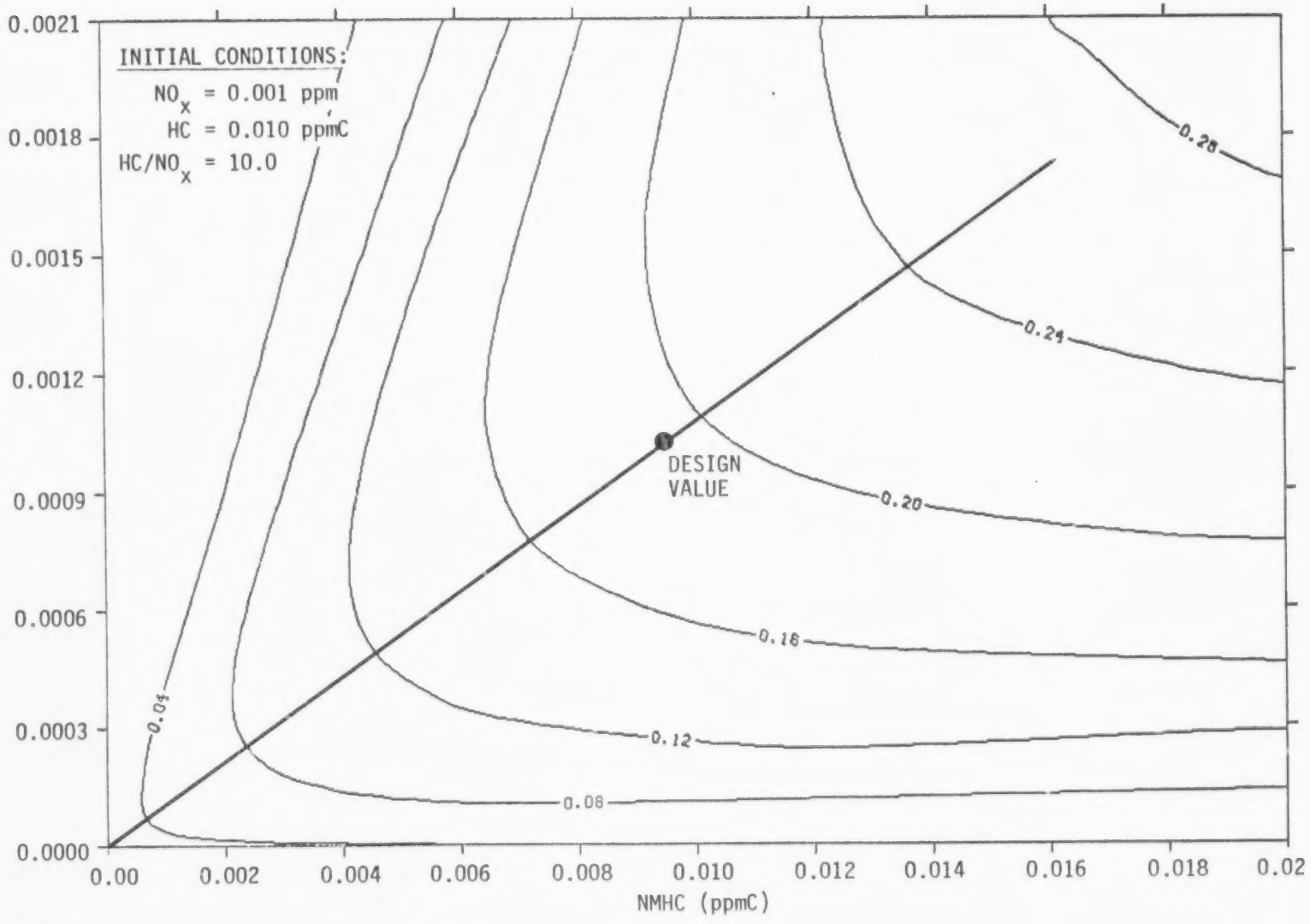
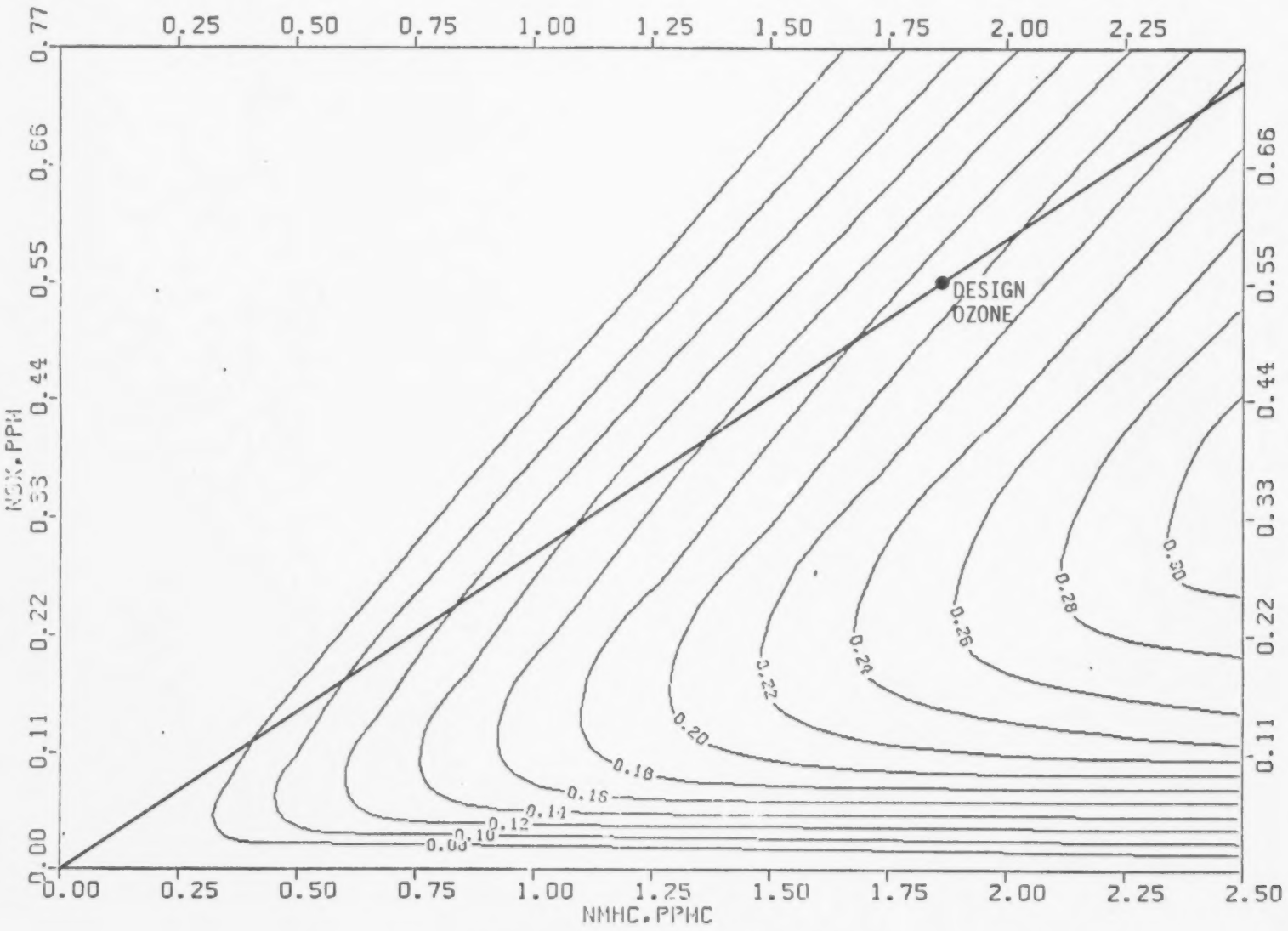
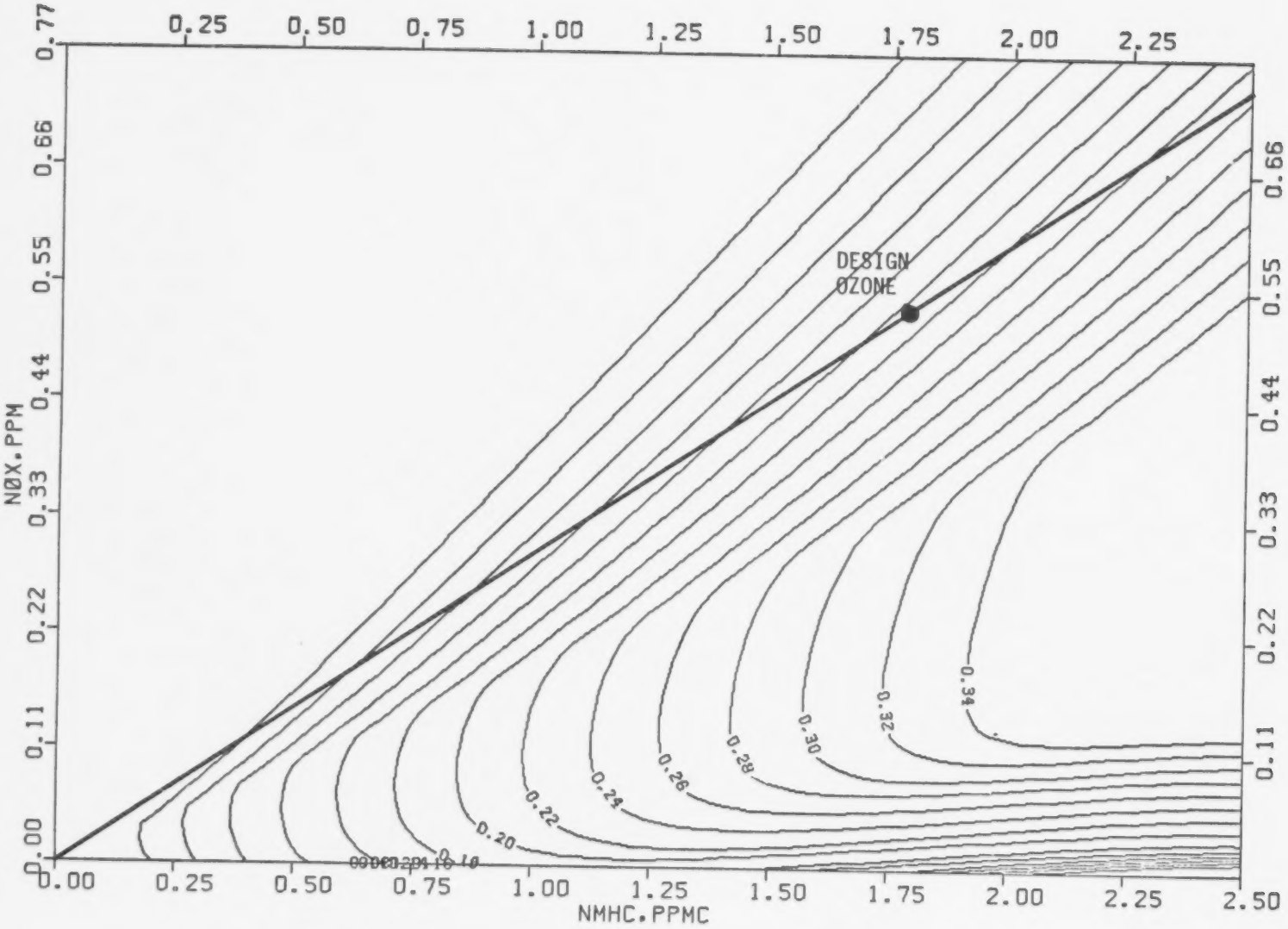


FIGURE 15. ISOPLETH FOR 26 JULY 1973: TRAJECTORY 1--HC/NO$_x$ RATIO = 10/1



(a) Regular City-Specific EKMA

FIGURE 16. LEVEL III TRAJECTORY FOR SAN FRANCISCO--26 JULY 1973



(b) City-Specific EKMA Using the Carbon-Bond Mechanism

FIGURE 16 (Concluded)

concentrations were usually between 1.3 and 1.9 ppmC. For the average 0600-to-0900-NMHC concentration, we assumed that the methane concentration was 1.6 ppmC. The calculated design HC/NO_x ratio for San Francisco is 3.3. This low value is similar to the low values estimated by de Mandel et al. (1979), who reported in their study that typical HC/NO_x ratios were between 1.2 and 1.7 for the five worst ozone episode days.

The emission rates presented in table 11 were taken from ARB (1976). However, information concerning hydrocarbon emissions reactivity is needed to utilize the Carbon-Bond Mechanism. Even though this information was not readily available, we decided to use the same reactivity as that of the LIRAQ model. This resulted in an OLE fraction of 18.1 percent, PAR fraction of 80.4 percent, and CARB fraction of 1.6 percent. Since the LIRAQ model does not contain any aromatics, we set the ARO fraction to zero. Without aromatics the hydrocarbon reactivity value used in this study may not reflect the true urban emissions mixture, nor does it reflect a typical reactivity for the use of the Carbon-Bond Mechanism.

The control strategy comparisons shown in table 10 reveal that the city-specific EKMA predictions using the standard EKMA chemistry most nearly parallel those obtained using the LIRAQ model. When the Carbon-Bond Mechanism is used, the sensitivity of ozone predictions to changes in emissions is greater.

5.2.2 Further Investigations

In this section, we describe the results of some additional analyses performed to assess the sensitivity of control strategy predictions using the EKMA. First, the sensitivity to the HC/NO_x ratio under particular conditions is examined. Second, the sensitivity of control estimates to particular trajectory path conditions is explored. Finally, an alternative method for generating isopleth diagrams and evaluating control strategies is presented.

In section 4.1.1, we indicated that the predicted peak ozone levels for trajectory 1, 26 July 1973, were insensitive to the assumed initial conditions. Likewise, the control predictions for this special case should be insensitive to the HC/NO_x ratio. As described earlier, the emissions input vectors were constructed from the LIRAQ emissions inventory. For the sensitivity study concerning the insignificance of the initial conditions (see table 9), we altered the emissions vectors to maintain constant contributions from the emissions regardless of the initial values or ratios of HC and NO_x. We also demonstrated that entire isopleth diagrams used with widely varying design HC/NO_x ratios can be

TABLE 11. INITIAL CONDITIONS USED IN THE LEVEL III EKMA CALCULATIONS FOR 26 JULY 1973 IN THE SAN FRANCISCO REGION

(a) Initial Conditions

Species	Transported Pollutants	
	Surface	Aloft
NO_x	0.0 ppm	0.0 ppm
NMOC	0.0 ppmC	0.0 ppmC
O_3	0.0 ppm	0.04 ppm

NO_2/NO_x = 0.25.
Hydrocarbon reactivity: standard OZIPP conditions.
Morning mixing height: 150 m at 0800 PDT.
Afternoon mixing height: 977 m at 1600 PDT.
0600 to 0900 hours HC/NO_x = 3.3.
0600 to 0900 hours NMOC = 0.4 ppmC.
0600 to 0900 hours NO_x = 0.12 ppm.
Design O_3 = 0.19 ppm at 1600 PDT near Livermore.

(b) County Emissions

County	ROC (tons/day)	NO_x (tons/day)	Area (km^2)	Density (kg/hr km^2)	
				ROC	NO_x
San Francisco	97.7	83.0	116.55	31.69	26.92
Alameda	187	131.0	1898.5	3.72	2.61

(c) Emissions Fraction

Time (PDT)	Trajectory	ROC Fractions	NO_x Fractions
0800-0900	San Francisco/Alameda	0.496	0.434
0900-1000	Alameda	0.104	0.0767
1000-1100	Alameda	0.104	0.0767
1100-1200	Alameda	0.104	0.0767
1200-1300	Alameda	0.104	0.0767
1300-1400	Alameda	0.104	0.0767
1400-1500	Alameda	0.104	0.0767
1500-1600	Alameda	0.104	0.0767

32R/14

constructed and can produce consistent results if the HC/NO_x ratio employed is the one upon which the emissions vector was constructed. Four key points result from the investigation of this special trajectory:

> The EKMA can still be used as a control strategy tool, provided that the special emissions input vectors and design HC/NO_x ratios are consistent.

> The observed HC/NO_x ratio is not needed.

> The underlying effective HC/NO_x ratio is found in the emissions inventory.

> The isopleth-derived control implications are directly related to the emissions themselves rather than to the results of typical applications (where the initial conditions of precursors dominate the model).

Two additional isopleth diagrams were constructed to illustrate the technique developed for trajectories (such as those we found in San Francisco) that are not sensitive to initial conditions. The base-case isopleth diagram chosen was the one shown earlier in figure 15 in which the initial condition HC/NO_x ratio used in the base trajectory (i.e., the 26 July 1973 trajectory originally shown in figure 1) is 10/1. As previously described, the design ozone value must be located on this HC/NO_x ratio line when this technique is used. The diagrams are shown in figures 17 and 18. The initial-condition base HC/NO_x ratio lines to be used for these diagrams are 1/1 and 100/1, respectively. These diagrams were constructed using the technique described earlier for showing insensitivity to initial conditions--that is, the emissions vectors were recomputed so that the contributions of emissions to the model concentrations in the base-case trajectory were all the same. The trajectory model results were presented earlier in table 9 and were discussed in section 4. The control implications of these additional diagrams, shown in table 12, demonstrate that consistent utilization of emissions inventory information produces consistent isopleth-derived results, provided that the proper HC/NO_x ratio (i.e., the ratio used to construct the emissions vector) is utilized with the design O_3 when initial conditions are not important.

Recall from chapter 3 that the OZIPM model (i.e., the Level II analysis) was applied to several other trajectories in addition to the basic 26 July 1973 trajectory that corresponds to the prototype conditions modeled using the LIRAQ. Two additional isopleths were developed for the trajectories shown in figures 3 and 5: trajectory 1 for 20 August 1973, and trajectory 2 for 24 July 1974, respectively. The two diagrams are shown in figures 19 and 20. The LIRAQ control scenarios were evaluated

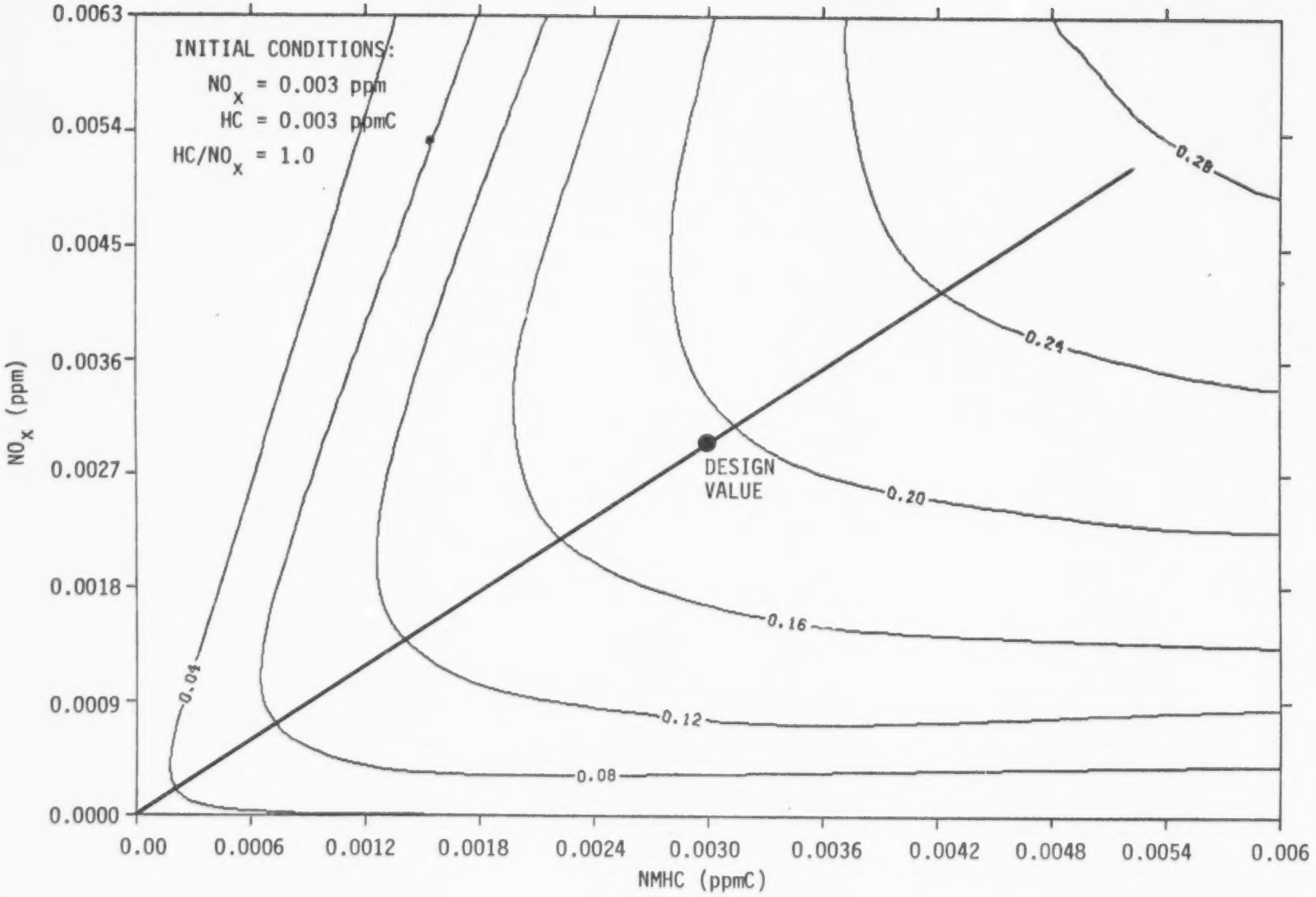


FIGURE 17. ISOPLETH FOR 26 JULY 1973: TRAJECTORY 1--HC/NO_x RATIO = 1/1

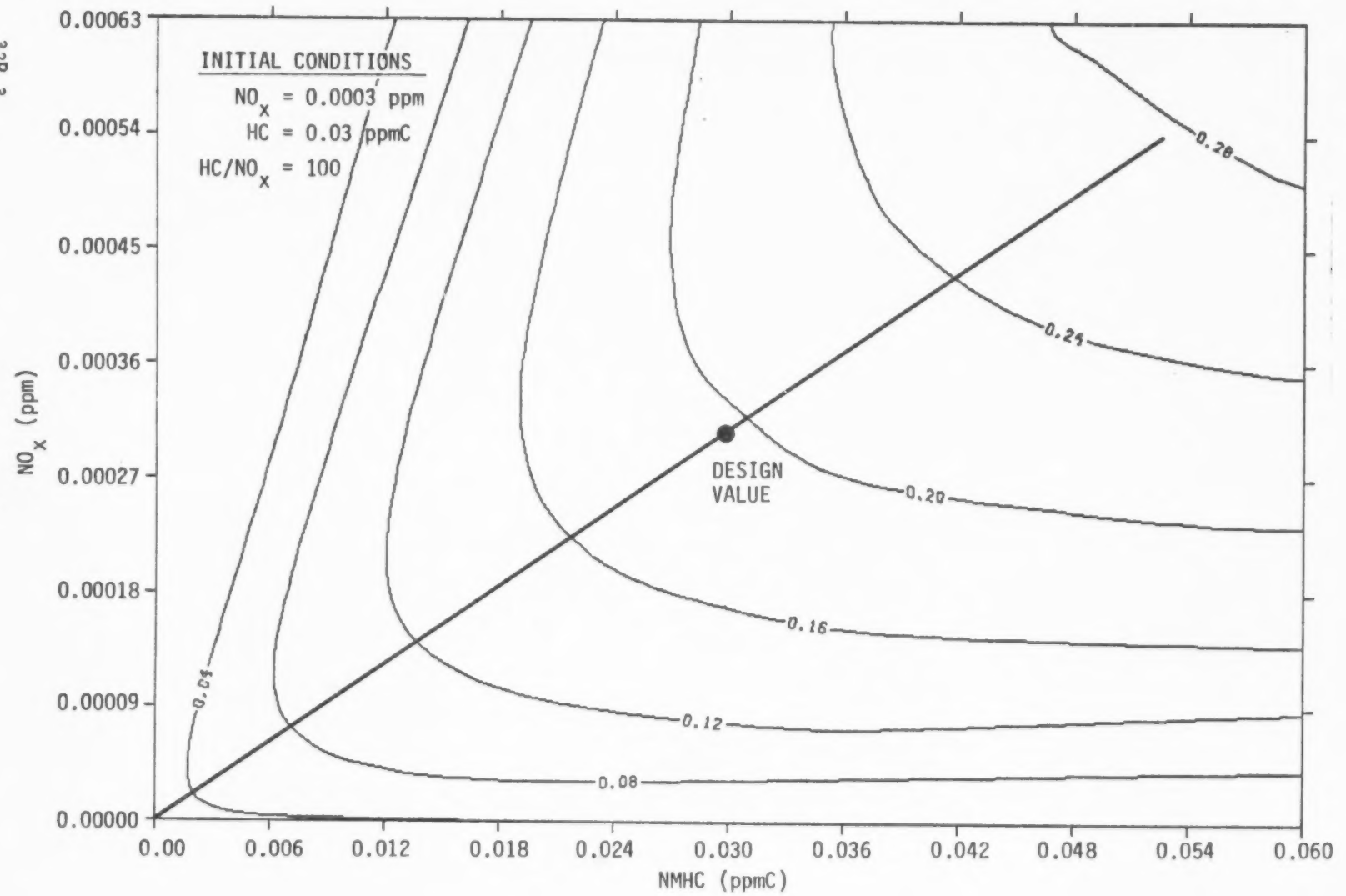


FIGURE 18. ISOPLETH FOR 26 JULY 1973: TRAJECTORY 1--HC/NO_x RATIO = 100/1

TABLE 12. SENSITIVITY OF CONTROL-STRATEGY EVALUATION TO HC/NO_x RATIO FOR TRAJECTORY 1--26 JULY 1973

Cases Studied	Reduction (percent) HC / NO_x								
	HC	0	20	40	60	80	40	80	0
	NO_x	0	0	0	0	0	20	40	40
OZIPM (Level II) (based on 0.189 max.) trajectory for 26 July 1973; HC/NO_x = 100		0.189	0.165	0.146	0.105	0.040	0.145	0.063	0.160
City-specific using OZIPM (based on 0.189 max.) 1975 trajectory for 26 July 1973; NC/NO_x = 1.0		0.189	0.169	0.142	0.098	0.036	0.143	0.060	0.160

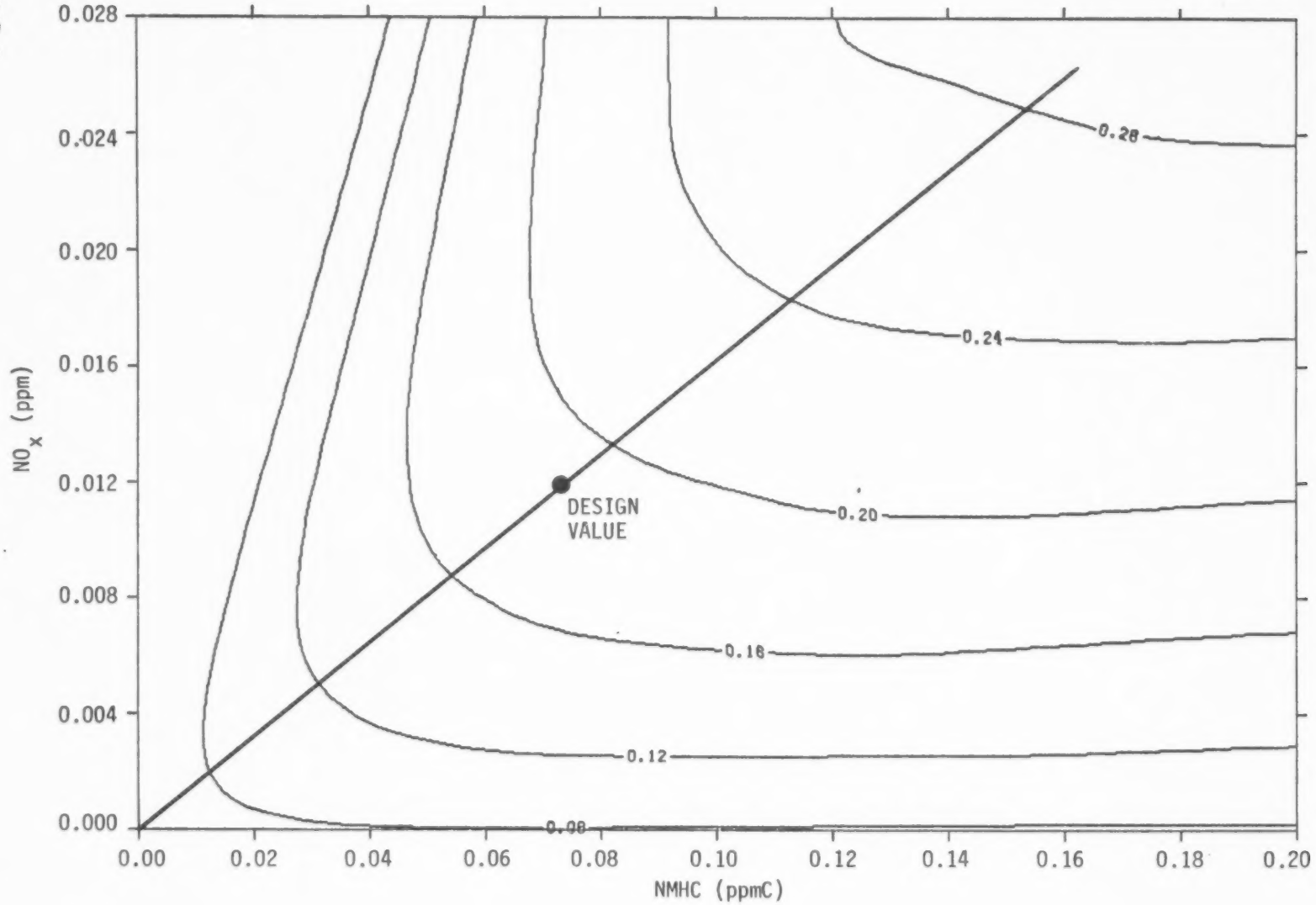


FIGURE 19. ISOPLETH FOR 20 AUGUST 1973: TRAJECTORY 1

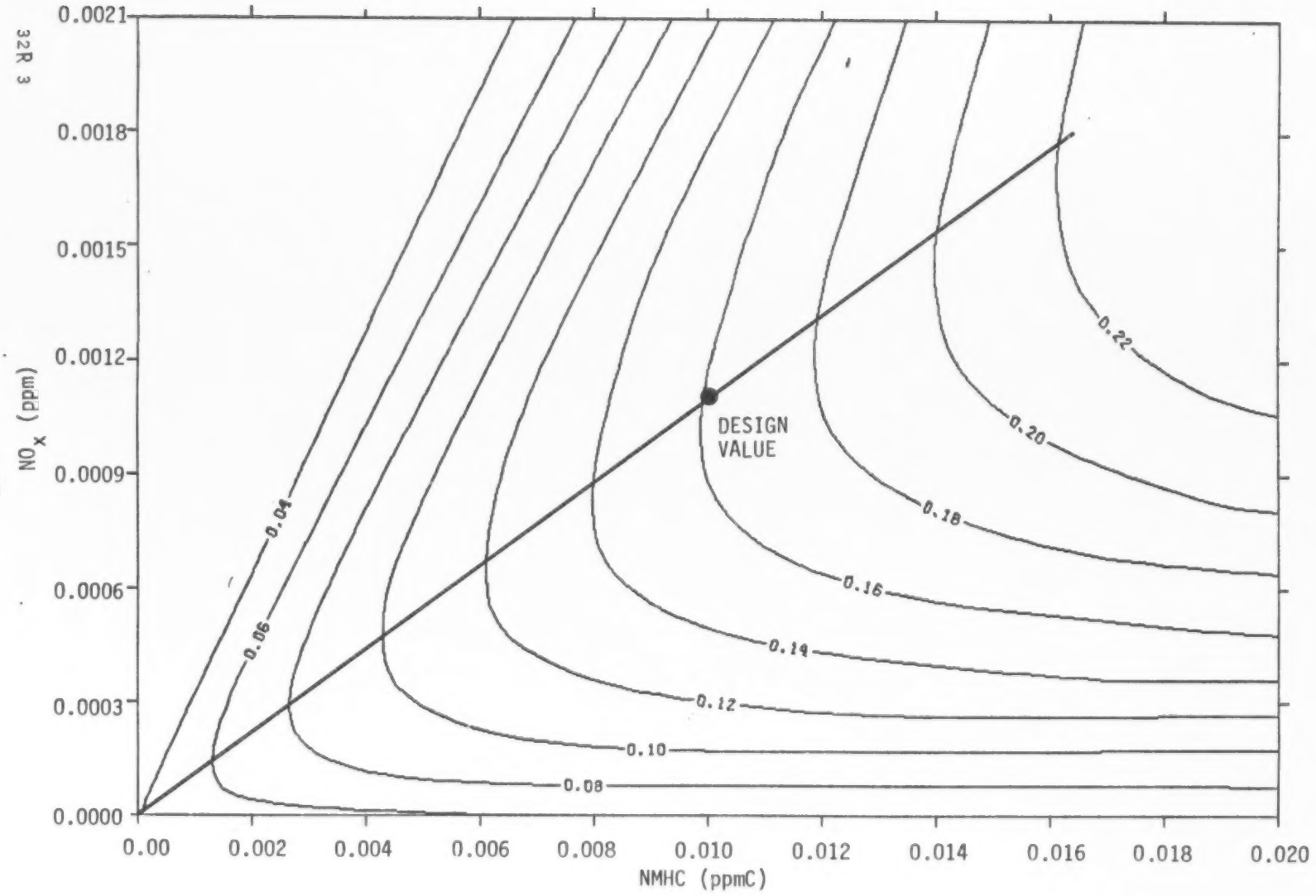


FIGURE 20. ISOPLETH FOR 24 JULY 1974: TRAJECTORY 2

using the EKMA technique with these diagrams. For these calculations, the HC/NO_x ratio corresponded to that of the assumed initial conditions, but an ozone maximum of 0.189 ppm was selected to compare more easily the EKMA predictions based on the different trajectories. Table 13 contains the control calculations for these two new trajectories, as well as those for the basic 26 July 1973 trajectory (i.e., trajectory 1). The results demonstrate that control estimates can be sensitive to trajectory path, as might be expected. Interestingly, some predictions using these new trajectories agree more closely with the LIRAQ results than do the trajectories previously discussed.

In the recent study by Whitten and Hogo (1981), a new type of EKMA isopleth was introduced that uses the emissions inventories for NO_x and HC as the ordinate and abscissa of the diagram. The (1,1) point of such a diagram corresponds to the trajectory simulation using the present emissions inventory. Figure 21 shows the isopleth of 26 July 1973 in which the (1,1) point is the trajectory shown in figure 1. The HC/NOx ratio to be used with the new diagram is the diagonal line through the (1,1) point. Using this HC/NO_x line and the 0.189 ppm design, O_3-value ozone predictions were computed using the regular procedures. The results are shown in table 14.

Note that the design ozone and the simulated ozone at the (1,1) point do not need to be the same. The new method is used exactly as the original EKMA except that the HC/NO_x ratio line through the (1,1) point is used in place of the observed 0600-to-0900-hour concentration ratio. Thus, the new method in effect substitutes the emissions inventory information for the 0600-to-0900-hour observed data. The similarity of these results to those of the regular city-specific isopleth shown in figure 15 is to be expected in this case because the initial conditions are not important. The intended advantages of using the new type of isopleth are the elimination of the initial HC/NO_x ratio data requirement. The initial conditions can be handled in one of two ways as can the concentrations aloft. In one method the concentrations are rolled back (or ahead) away from the (1,1) point of the diagram when the isopleth diagram is constructed. The initial conditions are thus treated as concentrations transported in the surface layer. In the other method, the initial conditions are still handled as surface-transported pollutants, but they are held constant over the entire isopleth diagram. Then, another diagram is constructed in which the expected future concentrations are held constant. This is actually the current method for handling present and future transported pollutants contained in the OZIPP computer code used in the Level III applications of the EKMA. Thus, the initial conditions may still be important, and their importance can be treated using this new method.

TABLE 13. SENSITIVITY OF CONTROL-STRATEGY EVALUATION TO TRAJECTORY PATH

Cases Studied	Reduction (percent) HC / NO_x	0 / 0	20 / 0	40 / 0	60 / 0	80 / 0	40 / 20	80 / 40	0 / 40
OZIPM (Level II) Trajectory 1 for 26 July 1973		0.189	0.161	0.145	0.102	0.036	0.141	0.062	0.160
City-specific using OZIPM (based on 0.189 max.) 1975 trajectory for 24 July 1974		0.189	0.162	0.127	0.070	<0.02	0.135	0.048	0.172
City-specific using OZIPM (based on 0.189 max.) 1975 trajectory for 20 August 1973		0.189	0.168	0.128	0.082	0.043	0.132	0.058	0.185
Average for 3 OZIPM runs		0.189	0.164	0.133	0.085	0.03	0.136	0.056	0.172

32R/14

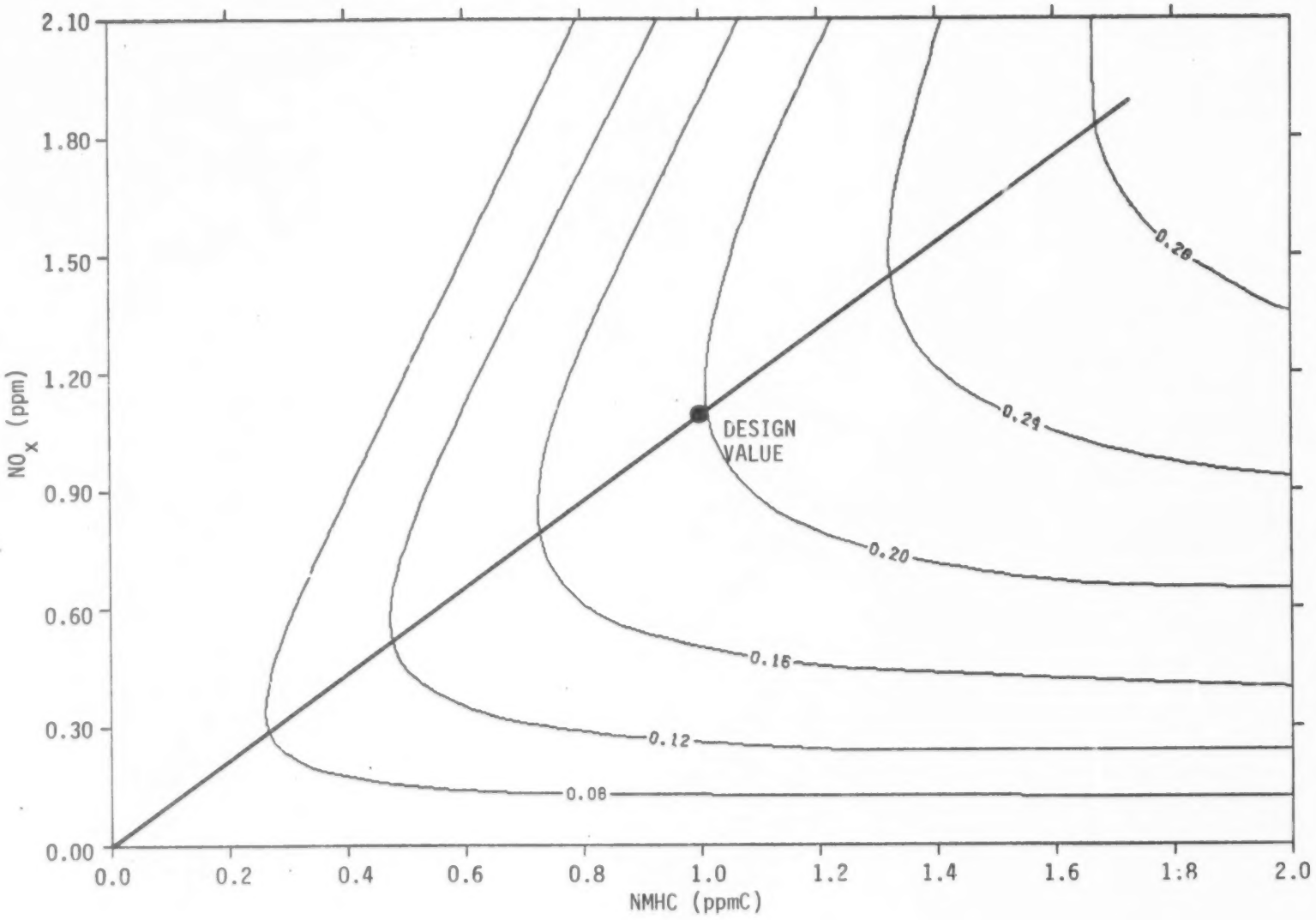


FIGURE 21. NEW-STYLE ISOPLETH (1,1) FOR 26 JULY 1973: TRAJECTORY 1

TABLE 14. CONTROL-STRATEGY COMPARISONS USING A NEW-STYLE ISOPLETH

Models Studied	Reduction (percent) HC / NO_x	0 / 0	20 / 0	40 / 0	60 / 0	80 / 0	40 / 20	80 / 40	0 / 40
LIRAQ predictions		0.189	0.140	0.082	0.069	0.055	0.119	0.064	0.233
OZIPM (Level II) Trajectory 1 for 26 July 1973; new-style isopleth		0.189	0.165	0.125	0.075	>0.02	0.132	0.063	0.163
OZIPM/CBM (Level II) Trajectory 1 for 26 July 1973; new-style isopleth		0.189	0.161	0.12	0.078	0.038	0.134	0.053	0.172

We have also used this new-style diagram with the new Carbon-Bond Mechanism, which was employed by Whitten and Hogo (1981). The diagram generated using the trajectory of 26 July 1973 with the CBM chemistry is presented in figure 22, and the control-scenario results are included in table 14. Although the CBM chemistry generates more simulated ozone than the regular EKMA chemistry for the (1,1) point, the control-scenario predictions (which are based on EKMA-style relative application to a single-design O_3) turn out to be quite similar except for the case of 80 percent HC/40 percent NO_x combined control.

5.3 SACRAMENTO APPLICATION

Part of the task of the original SAI Airshed Model study of the Sacramento region was to examine the effects of controlling mobile-source emissions (Reynolds et al., 1979). In order to perform the desired control simulations in the original study, the Sacramento region was rotated to form a special air quality control region (AQCR) in which the main highway runs in an east-west direction. Figure 23 shows this special modeling region. Meteorology for 24 August 1976 was used for the study. The wind fields for that day were also rotated in such a way that the predominant wind flow was from west to east, parallel to the main highway. The modeling region was expanded to contain 729 grid cells, each 3 km in length. The total region size is 81 km by 81 km. The original emissions inventory was increased to reflect the dimensions of the new region and a rotation scheme having the same emissions density as the original region.

Seven control strategies were defined, and airshed simulations were performed for these strategies on the rotated region. Table 15 shows the control strategies that were evaluated and the Airshed Model's predicted peak ozone concentration for each. Note that several of the control strategies cannot be easily simulated with the EKMA. Therefore, only the first two control strategies listed in table 15 (30 percent reduction in mobile-source HC and NO_x emissions, and 30 percent reduction in mobile-source HC only) were evaluated with the EKMA.

Because of the special rotation of the modeling region, new base-case evalulations had to be made using the SAI trajectory model, OZIPM/CBM, and city-specfic EKMA. As was done for the Sacramento simulations described in chapter 3, the trajectory path leading to the maximum ozone concentration was defined with the SAI trajectory model (shown in figure 24). From the trajectory model outputs, inputs for the OZIPM/CBM simulations were generated, and the inputs for the city-specific EKMA (OZIPP) model were then generated using the results of the OZIPM/CBM simulations. Tables 16 and 17 summarize the inputs for each model. Table 18 compares the predicted maximum ozone for the four models.

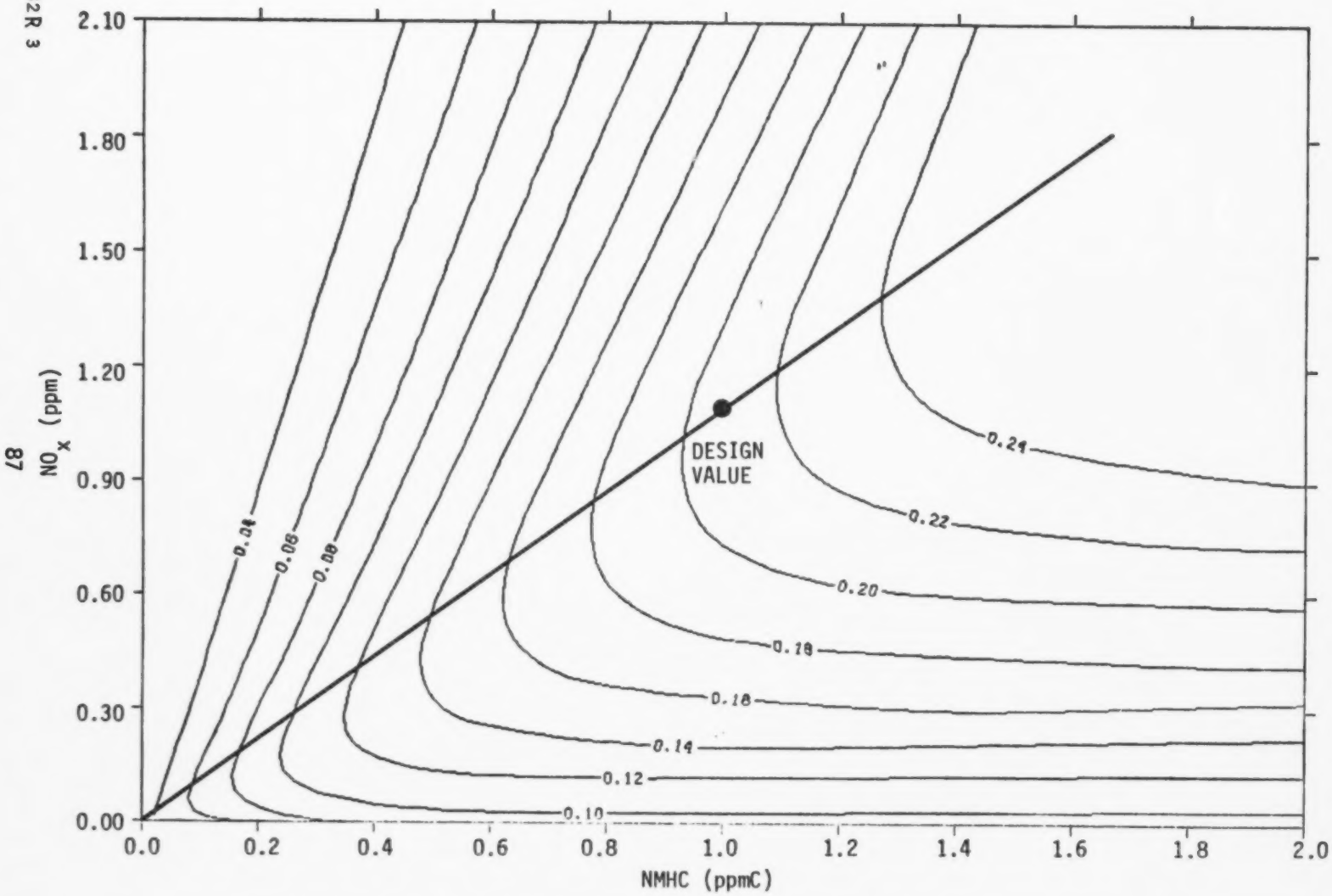


FIGURE 22. NEW-STYLE ISOPLETH (1,1) FOR 26 JULY 1973: TRAJECTORY 1 USING THE CARBON-BOND MECHANISM

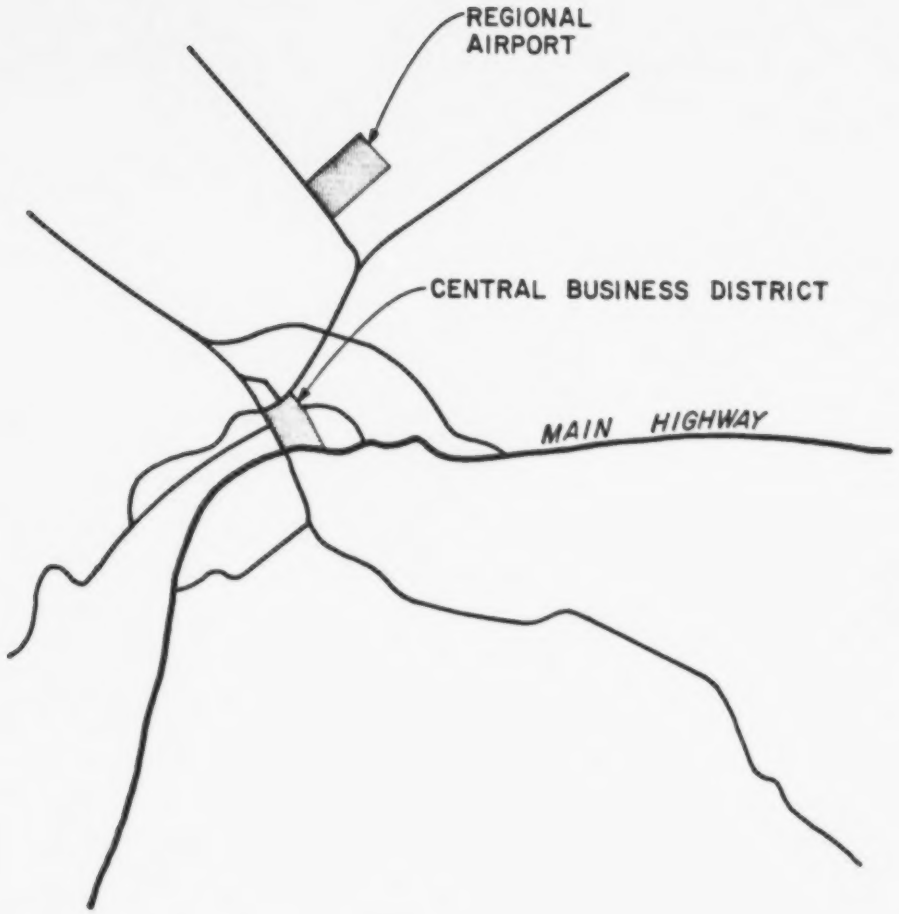


FIGURE 23. MAP OF THE HYPOTHETICAL URBAN AREA USED TO STUDY TRANSPORTATION CONTROL STRATEGIES

TABLE 15. SAI AIRSHED MODEL PREDICTED PEAK OZONE CONCENTRATIONS COMPUTED FOR DIFFERENT CONTROL STRATEGIES IN THE HYPOTHETICAL REGION (base-case predicted peak ozone = 17 pphm)

Control Strategy Simulation		Peak Ozone Predicted (pphm)
(1a)	Reduction of all mobile source emissions by 30 percent	15
(1b)	Reduction of mobile emissions of HC by 30 percent	13
(2a)	30 percent reduction in mobile emissions along a corridor parallel to prevailing wind	17
(2b)	30 percent reduction in mobile emissions along a corridor perpendicular to prevailing wind	17
(2c)	30 percent reduction in mobile emissions in the central business district	16
(3a)	Use of 3-hour running-average emissions	17
(3b)	Delaying of all emissions by 3 hours	10

32R/14

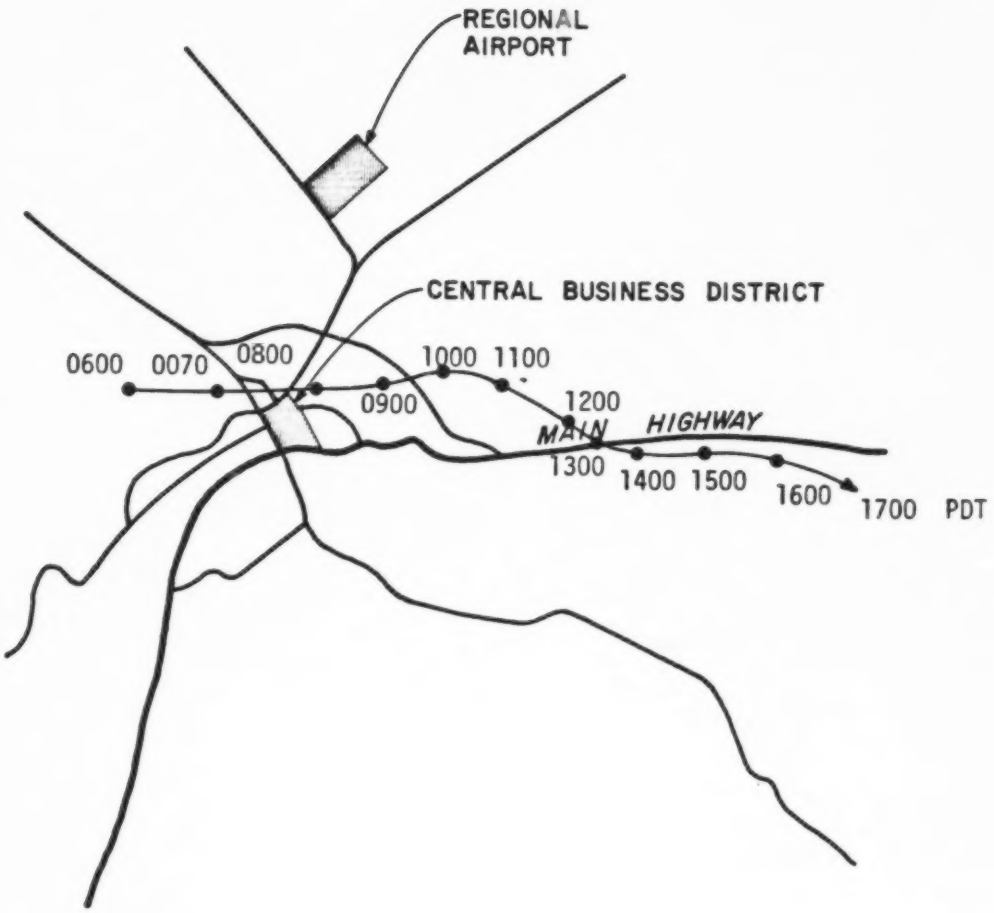


FIGURE 24. TRAJECTORY USED FOR THE CONTROL-STRATEGY RUNS (MODIFIED SACRAMENTO REGION)

TABLE 16. EMISSION RATES AND MIXING HEIGHTS USED IN EKMA APPLICATIONS TO HYPOTHETICAL REGION CONTROL STRATEGIES*

Time (PDT)	NO_x (ppm/hr)	HC (ppmC/hr)	Mixing Heights (meters)
0600	0.0133	0.039	50
0700	0.0641	0.3719	50
0800	0.0629	0.4171	100
0900	0.06958	0.493	150
1000	0.05804	0.2904	225
1100	0.0792	0.2239	300
1200	0.08836	0.1759	450
1300	0.0798	0.258	600
1400	0.098	0.2445	800
1500	0.0677	0.1116	800
1600	0.0099	0.01728	800
1700	--	--	800

* Taken from the SAI trajectory model calculations.

TABLE 17. TRAJECTORY MODEL OUTPUTS USED AS INPUTS FOR THE EKMA SIMULATIONS

(a) Initial Conditions and Hydrocarbon Reactivities Used in the OZIPM/CBM Control Base-Case Run (starting time = 0600 PDT)*

Species	Transported Pollutants	
	Surface	Aloft
NO_x	0.003 ppm	0.003 ppm
HC	0.057 ppmC	0.055 ppmC
O_3	0.019 ppm	0.026 ppm

Hydrocarbon Reactivities

Species	Surface	Aloft	Emissions
OLE	0.014	0.009	0.041
PAR	0.616	0.607	0.698
ARO	0.282	0.257	0.239
CARB	0.088	0.105	0.023

(b) Initial Conditions Used in City-Specific EKMA Calculations of Hypothetical Control Runs (starting time = 0800 PDT)

Species	Transported Pollutants	
	Surface	Aloft
NO_x	0.041 ppm	0.003 ppm
HC	0.248 ppmC	0.055 ppmC
O_3	0.009 ppm	0.026 ppm

NO_2/NO_x = 0.556.
Propylene reactivity = 0.25.
Dilution: initial mixing height = 100 m;
final mixing height = 800 m.

* Taken from the SAI trajectory model calculation.

32R/14

TABLE 18. COMPARISON OF MAXIMUM PREDICTED OZONE FOR THE SAI AIRSHED, SAI TRAJECTORY, OZIPM/CBM, AND CITY-SPECIFIC EKMA MODELS: BASE-CASE CONDITIONS USED FOR THE CONTROL-STRATEGIES STUDY OF THE HYPOTHETICAL REGION

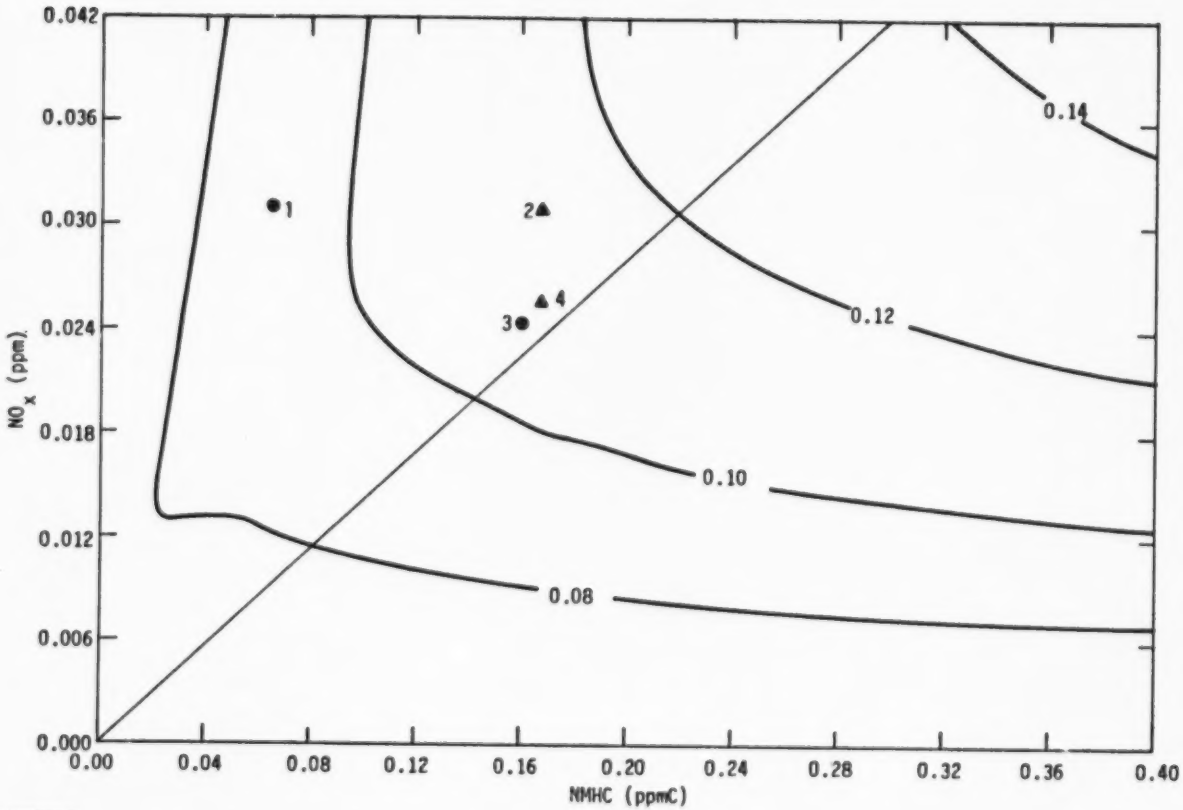
Model	Maximum O_3 (ppm)
SAI Airshed	0.17
SAI trajectory	0.12
OZIPM/CBM	0.12
City-specific EKMA	0.13

The comparison of predicted maximum ozone shows that the trajectory model and the two EKMA models give similar results, whereas the Airshed Model prediction is approximately 40 percent higher than that of the trajectory model. The special "rotated" emissions grid constructed for the study turned out not to be compatible with the SAI trajectory model computer code. Several attempts to construct a compatible emissions grid failed to produce one that reproduced in the trajectory model the concentrations that were seen in the original study. Since the precursor concentrations were low in the trajectory model simulations, low ozone values were expected. Unfortunately, time and cost constraints precluded the resolution of this emissions inventory problem.

The two control strategies were evaluated directly with SAI trajectory model simulations reflecting the assumed emission reductions. For the EKMA applications, isopleths were generated to evaluate the strategies. Figure 25 shows the isopleth generated for the city-specific EKMA application. The regional, initial HC/NO_x ratio of 7.2 is taken from Reynolds, et al. (1979). The initial HC/NO_x ratio, determined from the initial conditions for this specific trajectory is approximately 6/1. However, we used the HC/NO_x ratio of 7.2 because this value was derived for the EKMA as it is more normally applied. Since a 30 percent reduction was made in mobile emissions only, we needed to determine the reduction in total emissions (sum of mobile and stationary sources). From the Airshed Model emissions inventory containing the reduced mobile emissions and the trajectory path, we found the emissions for each hour along the trajectory path (see table 19). From the new emissions rates, we determined the level of control of HC and NO_x emissions from all sources to be reductions of 19.6 percent HC and 16.3 percent NO_x. Since the SAI Airshed Model and the SAI trajectory model did not predict similar ozone maximums, we decided to use the ozone maximum of 0.12 ppm predicted by the trajectory model as the design ozone value.

The EKMA predictions resulting from application of the two control strategies are presented in table 20. Controlling of HC mobile emissions only shows a 20 percent difference in predicted maximum ozone between the trajectory model and the city-specific EKMA model. This discrepancy appears to be a result of the different chemistry used in the two models because the CBM-EKMA simulation, with the same inputs as those of the city-specific EKMA run, predicted an ozone maximum much closer to that of the trajectory model.

Further investigations were made using Level III EKMA guidelines. From the initial conditions presented in table 21, and from emissions rates of ARB (1979), we generated two diagrams (one using the standard EKMA chemistry, the other using Carbon-Bond chemistry). For the CBM isopleth we used the same hydrocarbon reactivity as is presented in table 17. The isopleth diagram generated using the standard EKMA chemistry is



NOTES:

1) SAI trajectory model prediction (30 percent reduction in mobile emissions of HC only)
2) EKMA prediction (30 percent reduction in mobile emissions of HC only)
3) SAI trajectory model prediction (30 percent reduction in mobile emissions of both HC and NO_x)
4) EKMA prediction (30 percent reduction in mobile emissions of both HC and NO_x)

FIGURE 25. CITY-SPECIFIC EKMA ISOPLETH FOR THE CONTROL-STRATEGY CALCULATIONS

TABLE 19. CONTROL-STRATEGY STUDY TOTAL EMISSIONS RESULTING FROM A 30 PERCENT REDUCTION IN MOBILE HC AND NO_x EMISSIONS

Time (PDT)	NO_x (ppm/hr)	HC (ppmC/hr)
0600	1.004	0.0384
0700	0.0463	0.2882
0800	0.0455	0.3076
0900	0.052	0.3808
1000	0.0456	0.2327
1100	0.0694	0.1826
1200	0.0803	0.184
1300	0.0688	0.2097
1400	0.0875	0.1952
1500	0.0622	0.0895
1600	0.0088	0.0163
1700	--	--

32R/14

TABLE 20. COMPARISON OF MAXIMUM OZONE PREDICTIONS BETWEEN THE TRAJECTORY MODEL, OZIPM/CBM, AND CITY-SPECIFIC EKMA WITH DIFFERENT CONTROL SCENARIOS (design O_3 = 0.12 ppm)

Model	Predicted O_3-- 30 Percent Reduction in Mobile Emissions of HC and NO_x (ppm)	Predicted O_3-- 30 Percent Reduction in Mobile Emissions of HC Only (ppm)
Trajectory model	0.103 (-14%)	0.09 (-25%)
OZIPM/CBM	0.097 (-19%)	0.086 (-28%)
City-specific EKMA	0.108 (-10%)	0.114 (-5%)
Level III EKMA	0.104 (-13%)	0.105 (-13%)
Level III EKMA using CBM I	0.10 (-17%)	0.084 (-30%)
Level III EKMA using CBM II	0.101 (-16%)	0.082 (-32%)

32R/14

TABLE 21. INITIAL CONDITIONS USED IN THE LEVEL III EKMA CALCULATIONS FOR HYPOTHETICAL REGION FOR 24 AUGUST 1976 METEOROLOGY (emissions based on Sacramento County for 1976)

(a) Initial Conditions

Species	Transported Pollutants	
	Surface	Aloft
NO_x	0.0 ppm	0.0 ppm
NMOC	0.0 ppmC	0.0 ppmC
O_3	0.0 ppm	0.2 ppm

NO_2/NO_x = 0.25.
Hydrocarbon reactivity: standard OZIPP conditions.
Morning mixing height: 150 m at 0800 PDT.
Afternoon mixing height: 800 m at 1400 PDT.
0600 to 0900 hour HC/NO_x = 7.2.
0600 to 0900 hour NMOC = 0.248 ppmC.
0600 to 0900 hour NO_x = 0.035 ppm.
Design O_3 = 0.12 ppm at 1700 PDT.

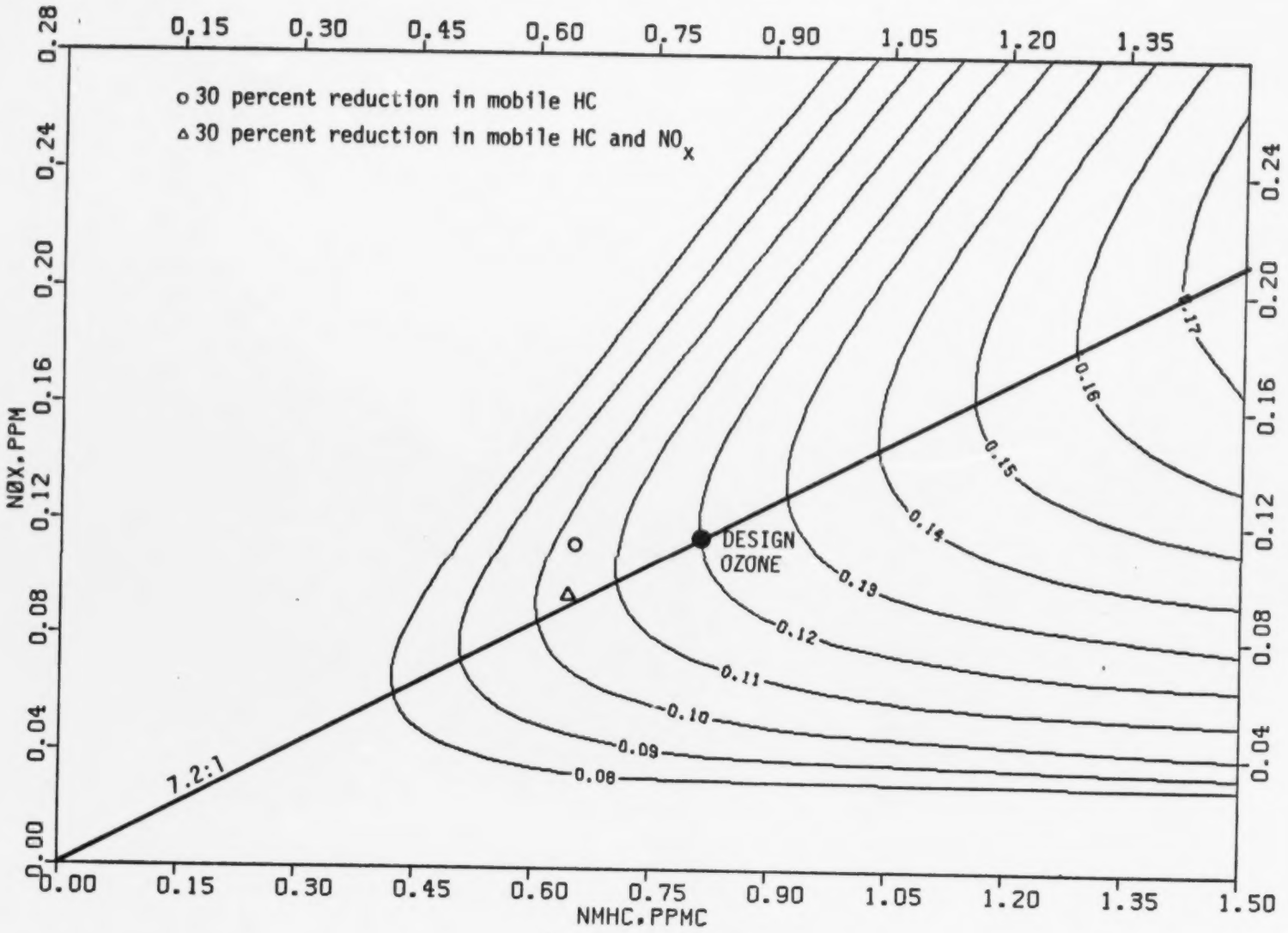
(b) County Emissions

County	ROC (tons/day)	NO_x (tons/day)	Area (km^2)	Density (kg/hr km^2)	
				ROC	NO_x
Sacramento	119.7	70.9	2525.24	1.79	1.29

(c) Emissions Fraction

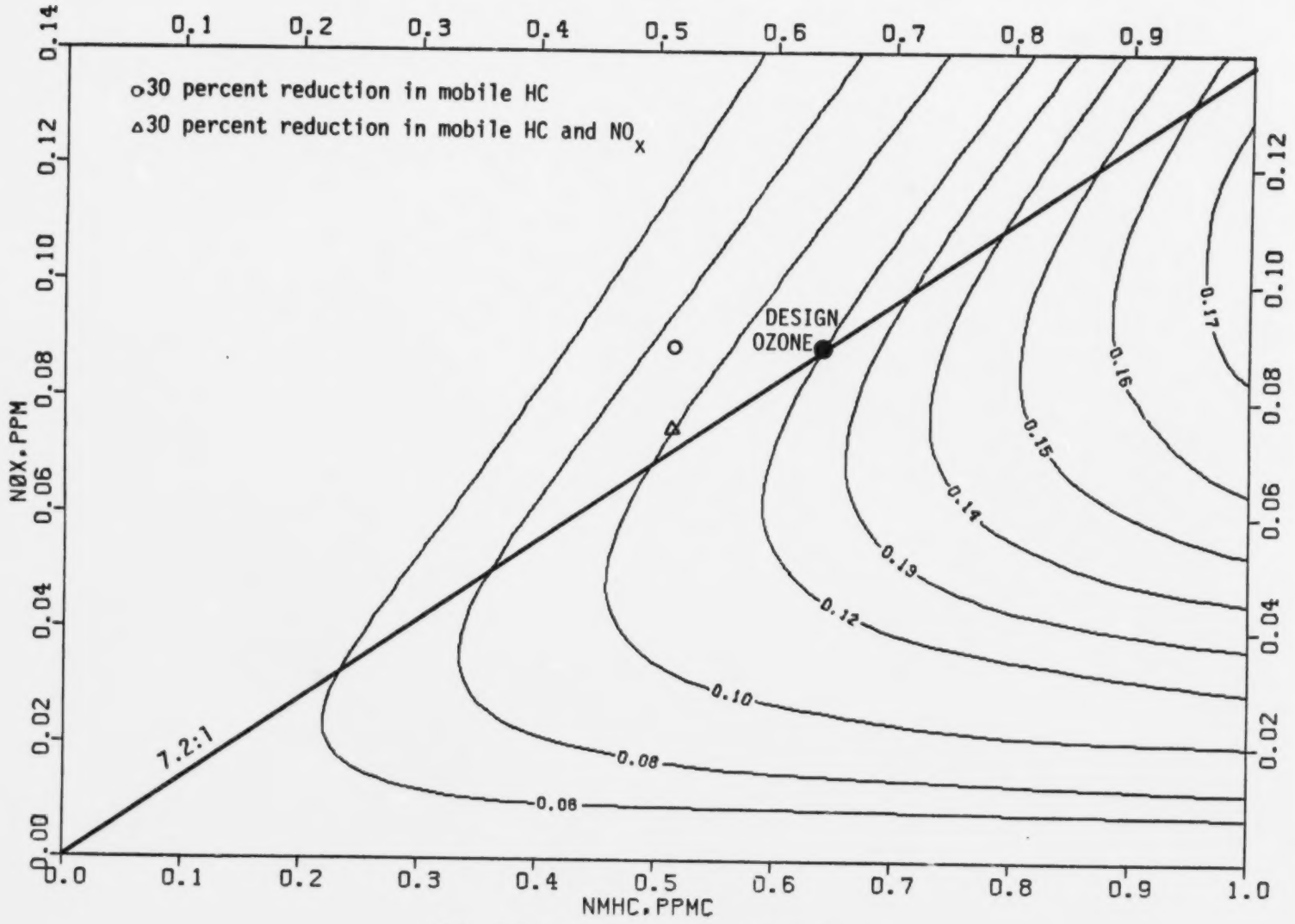
Time (PDT)	Trajectory	ROC Fractions	NO_x Fractions
0800-0900	Sacramento	0.081	0.130
0900-1000	Sacramento	0.081	0.130
1000-1100	Sacramento	0.081	0.130
1100-1200	Sacramento	0.081	0.130
1200-1300	Sacramento	0.081	0.130
1300-1400	Sacramento	0.081	0.130
1400-1500	Sacramento	0.081	0.130
1500-1600	Sacramento	0.081	0.130

shown in figure 26(a); the isopleth diagram with Carbon-Bond chemistry is shown in figure 26(b). The ozone predictions using the two diagrams are shown in table 20. For the 30 percent control of mobile emissions of HC, the Level III CBM-EKMA using both the old and new versions of the Carbon-Bond Mechanism [figures 26(b) and 26(c] predicts a lower ozone value than the standard Level III EKMA, as was true for the case that compared the CBM-EKMA with the city-specific EKMA. Thus, we see that the standard EKMA chemistry is less responsive to hydrocarbon controls. Yet, when both HC and NO_x emissions are reduced, the standard EKMA models (city-specific and Level-III) and the carbon-based trajectory model and OZIPM/CBM all give similar results.



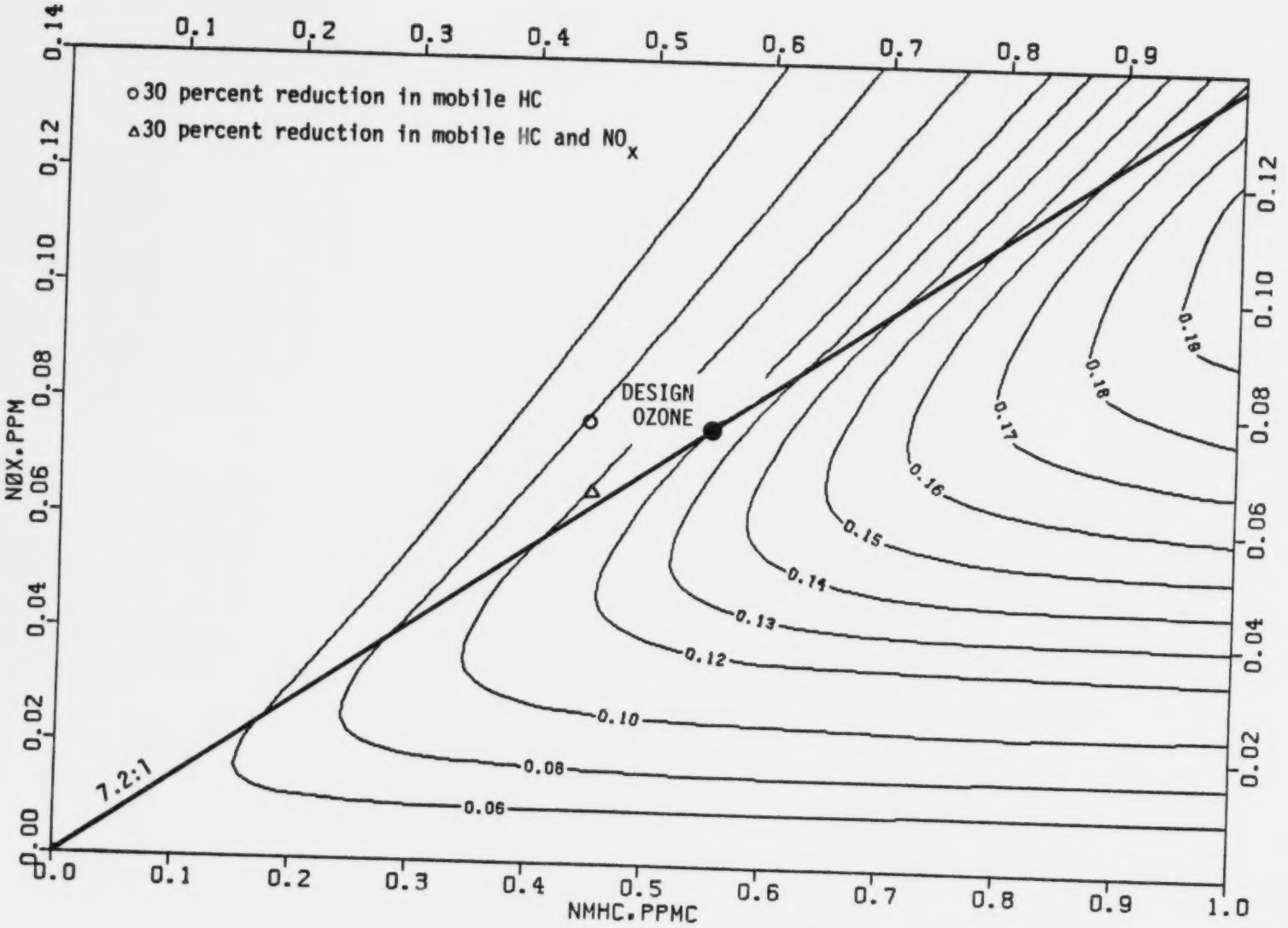
(a) Regular EKMA

FIGURE 26. LEVEL III TRAJECTORY FOR HYPOTHETICAL REGION: 24 AUGUST 1976



(b) Using the Carbon-Bond I Mechanism

FIGURE 26 (Continued)



(c) Using the Carbon-Bond II Mechanism

FIGURE 26 (Concluded)

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